

INVENTOR SEARCH

=> fil capl; d que l113; d que l116; s l113,l116
FILE 'CAPLUS' ENTERED AT 16:09:57 ON 02 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 2 Feb 2007 VOL 146 ISS 7
FILE LAST UPDATED: 1 Feb 2007 (20070201/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

L106	14460	SEA	FILE=CAPLUS	ABB=ON	KIM M?/AU
L107	25330	SEA	FILE=CAPLUS	ABB=ON	PARK J?/AU
L108	4144	SEA	FILE=CAPLUS	ABB=ON	CHUNG Y?/AU
L109	11169	SEA	FILE=CAPLUS	ABB=ON	CHOI J?/AU
L110	29440	SEA	FILE=CAPLUS	ABB=ON	LEE H?/AU
L111	8289	SEA	FILE=CAPLUS	ABB=ON	CHOI Y?/AU
L112	23463	SEA	FILE=CAPLUS	ABB=ON	KIM D?/AU
L113	1	SEA	FILE=CAPLUS	ABB=ON	L106 AND L107 AND L108 AND L109 AND L110 AND L111 AND L112

L17	150091	SEA	FILE=CAPLUS	ABB=ON	ALCOHOLS/CT
L19	18354	SEA	FILE=CAPLUS	ABB=ON	L17(L) PREP/RL
L20	136	SEA	FILE=CAPLUS	ABB=ON	L19(L) "S"/OBI
L22	23387	SEA	FILE=CAPLUS	ABB=ON	"RESOLUTION (SEPARATION)" +OLD/CT
L28	995	SEA	FILE=CAPLUS	ABB=ON	DYNAMIC/OBI (L) KINETIC/OBI
L29	226	SEA	FILE=CAPLUS	ABB=ON	L28(L) L22
L35	3653	SEA	FILE=CAPLUS	ABB=ON	CHIRAL/OBI (L) (ALCOHOL/OBI OR ALCS/OBI)

L106	14460	SEA	FILE=CAPLUS	ABB=ON	KIM M?/AU
L107	25330	SEA	FILE=CAPLUS	ABB=ON	PARK J?/AU
L108	4144	SEA	FILE=CAPLUS	ABB=ON	CHUNG Y?/AU
L109	11169	SEA	FILE=CAPLUS	ABB=ON	CHOI J?/AU
L110	29440	SEA	FILE=CAPLUS	ABB=ON	LEE H?/AU
L111	8289	SEA	FILE=CAPLUS	ABB=ON	CHOI Y?/AU
L112	23463	SEA	FILE=CAPLUS	ABB=ON	KIM D?/AU
L114	8708	SEA	FILE=CAPLUS	ABB=ON	(L106 AND (L107 OR L108 OR L109 OR L110 OR L111 OR L112)) OR (L107 AND (L108 OR L109 OR L110 OR L111 OR L112)) OR (L108 AND (L109 OR L110 OR L111 OR L112)) OR (L109 AND (L110 OR L111 OR L112)) OR (L110 AND (L111 OR L112))

OR (L111 AND L112)
 L116 17 SEA FILE=CAPLUS ABB=ON L114 AND (L29 OR L35 OR L20)

L117 17 (L113 OR L116)

=> fil casrea; d que nos 197
 FILE 'CASREACT' ENTERED AT 16:10:08 ON 02 FEB 2007
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 28 Jan 2007 VOL 146 ISS 5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*      CASREACT now has more than 10 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
L14      152839 SEA FILE=REGISTRY ABB=ON RU/ELS
L24      1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
L25      1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
L59      335 SEA FILE=CASREACT ABB=ON KIM M?/AU
L60      448 SEA FILE=CASREACT ABB=ON PARK J?/AU
L61      212 SEA FILE=CASREACT ABB=ON CHUNG Y?/AU
L62      255 SEA FILE=CASREACT ABB=ON CHOI J?/AU
L63      702 SEA FILE=CASREACT ABB=ON LEE H?/AU
L64      126 SEA FILE=CASREACT ABB=ON CHOI Y?/AU
L65      530 SEA FILE=CASREACT ABB=ON KIM D?/AU
L67      72677 SEA FILE=CASREACT ABB=ON STEREOSELECTIVE/NTE
L68      30236 SEA FILE=REGISTRY ABB=ON L14 AND CASREACT/LC
L69      8227 SEA FILE=CASREACT ABB=ON L68/CAT
L70      267 SEA FILE=CASREACT ABB=ON L24/CAT OR L25/CAT
L73      76833 SEA FILE=CASREACT ABB=ON (L69 OR L70 OR L67)
L76      STR
L82      SCR 1149
L87      3195 SEA FILE=CASREACT SUB=L73 SSS FUL L76 AND L82 ( 20816 REACTIONS
)
L88      3187 SEA FILE=CASREACT ABB=ON L87/COMPLETE
L94      207 SEA FILE=CASREACT ABB=ON (L59 AND (L60 OR L61 OR L62 OR L63
OR L64 OR L65)) OR (L60 AND (L61 OR L62 OR L63 OR L64 OR L65))
OR (L61 AND (L62 OR L63 OR L64 OR L65)) OR (L62 AND (L63 OR
L64 OR L65)) OR (L63 AND (L64 OR L65)) OR (L64 AND L65)
L95      13 SEA FILE=CASREACT ABB=ON L94 AND L88 AND L67
```

L96 14 SEA FILE=CASREACT ABB=ON L94 AND L88 AND (L69 OR L70)
 L97 13 SEA FILE=CASREACT ABB=ON L95 AND L96

=> dup rem 197,1117

FILE 'CASREACT' ENTERED AT 16:10:19 ON 02 FEB 2007
 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CAPLUS' ENTERED AT 16:10:19 ON 02 FEB 2007
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

PROCESSING COMPLETED FOR L97

PROCESSING COMPLETED FOR L117

L118 24 DUP REM L97 L117 (6 DUPLICATES REMOVED)

ANSWERS '1-13' FROM FILE CASREACT

ANSWERS '14-24' FROM FILE CAPLUS

=> d ibib ed abs fhit

'ED' IS NOT A VALID FORMAT

REENTER DISPLAY FORMAT FOR ALL FILES (FILEDEFAULT):end

=> d ibib abs fhit 1-13; d ibib ed abs hitind 14-24

L118 ANSWER 1 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 142:197677 CASREACT Full-text
 TITLE: Method of preparation of optically active alcohols
 INVENTOR(S): Kim, Mahn-Joo; Park, JaiWook;
 Chung, Yong Il; Choi, Jun Ho;
 Lee, Han Ki; Choi, Yoon Kyung;
 Kim, Daeho
 PATENT ASSIGNEE(S): Postech Foundation, S. Korea; Posco
 SOURCE: PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

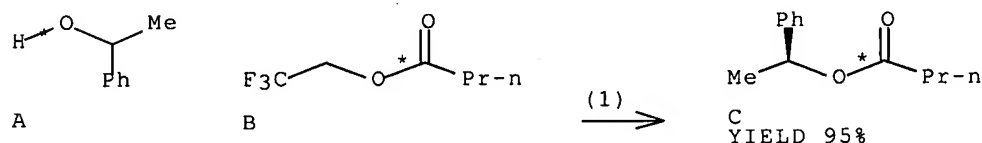
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005009935	A1	20050203	WO 2003-KR1494	20030725
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003247201	A1	20050214	AU 2003-247201	20030725
US 2007015943	A1	20070118	US 2006-565829	20060825
PRIORITY APPLN. INFO.:			WO 2003-KR1494	20030725

OTHER SOURCE(S): MARPAT 142:197677

AB The present invention relates to a method for preparing chiral alc. having optical activity. More specifically, the present invention relates to a

method for preparing (S)-chiral alc. with a high yield and a high optical purity by mixing achiral substrates such as racemic alc. or ketone with a combination of metal catalyst and protein hydrolase to perform a dynamic kinetic resolution reaction. Thus, to a Schlenk flask, 3.7 mg (Ph₄C₅NHCHMe₂)Ru(CO)₂Cl and 18 μ L t-BuOK solution (1 M in THF) was added and dried under the reduced pressure, followed by adding 1 mL toluene and then the resulting mixture was agitated for 1 h. After the toluene was removed under the reduced pressure, 9 mg stabilized subtilisin, 31.8 mg Na₂CO₃, 18 μ L 1-phenylethanol, 39 μ L 2,2,2-trifluoroethyl butyrate, and 0.5 mL THF were added and the mixture was agitated at room temperature for 3 days. After termination of the reaction, catalyst was filtered, the obtained filtered solution was concentrated and separated using column chromatog. (silica gel, Et acetate/ hexane = 4:1) to give (S)-1-phenylethyl butyrate (I) % yield and optical purity 92% ee. (S)-(-)-phenylethanol was obtained by adding I and 2 equiv of K₂CO₃ to 80% methanol solution and hydrolyzing at room temperature

RX(1) OF 29 A + B ==> C...



RX(1)

STAGE(1)

RGT D 865-47-4 t-BuOK
 CAT 470688-18-7 Ruthenium,
 dicarbonylchloro[(1,2,3,4,5- η)-1-[(1-methylethyl)amino]-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]-
 SOL 109-99-9 THF, 108-88-3 PhMe
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 1 hour, room temperature

STAGE(2)

RCT A 98-85-1, B 371-27-7
 RGT E 497-19-8 Na₂CO₃
 CAT 9014-01-1 Subtilisin
 SOL 109-99-9 THF
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 72 hours, room temperature

PRO C 161024-76-6

NTE stereoselective

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 2 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 2
 ACCESSION NUMBER: 140:321067 CASREACT Full-text
 TITLE: Aminocyclopentadienyl ruthenium complexes as
 racemization catalysts for dynamic kinetic resolution

of secondary alcohols at ambient temperature

AUTHOR(S): Choi, Jun Ho; Choi, Yoon Kyung;
Kim, Yu Hwan; Park, Eun Sil; Kim, Eun Jung; Kim,
Mahn-Joo; Park, Jaiwook

CORPORATE SOURCE: National Research Laboratory of Chirotechnology,
Department of Chemistry, Division of Molecular and
Life Sciences, Pohang University of Science and
Technology, Pohang, 790-784, S. Korea

SOURCE: Journal of Organic Chemistry (2004), 69(6), 1972-1977
CODEN: JOCEAH; ISSN: 0022-3263.

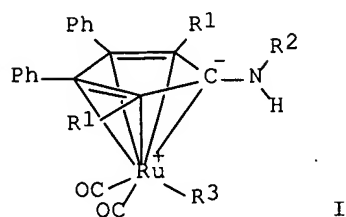
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

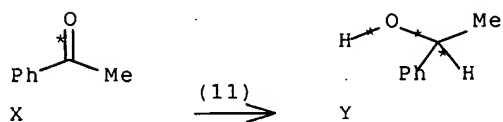
GI

got it.



AB Aminocyclopentadienyl ruthenium complexes I [R1 = Ph; R2 = *i*-Pr (II), *n*-Pr, *t*-Bu, Ph, 4-O₂NC₆H₄, 4-ClC₆H₄, 4-MeOC₆H₄, 4-Me₂NC₆H₄; R3 = Cl; R1 = Me; R2 = *i*-Pr (III), Ph; R3 = Cl] which can be used as room-temperature racemization catalysts with lipase in the dynamic kinetic resolution (DKR) of secondary alcs., were synthesized from iminocyclopenta-2,4-dienes, Ru₃(CO)₁₂, and CHCl₃. The racemization of (*S*)-4-phenyl-2-butanol showed that III was the most active catalyst, although the difference decreased in the DKR. II was used in the DKR of various alcs. such as allylic alcs., alkynyl alcs., diols, hydroxy esters, and chlorohydrins, which were successfully transformed to chiral acetates. Mechanistic studies for the catalytic racemization, indicated that ruthenium hydride I [R1 = Ph; R2 = *i*-Pr; R3 = H (IV)] was the key species in the reaction. IV was the major organometallic species in the racemization of (*S*)-1-phenylethanol with II and potassium *tert*-butoxide. In a sep. experiment, (*S*)-1-phenylethanol was racemized catalytically by IV in the presence of acetophenone.

RX(11) OF 59 X ==> Y...



RX(11) RCT X 98-86-2

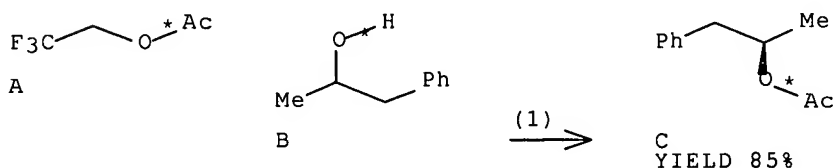
PRO Y 98-85-1
 CAT 600136-37-6 Ruthenium, dicarbonylhydro[(1,2,3,4,5-
 η)-1-[(1-methylethyl)amino]-2,3,4,5-tetraphenyl-2,4-
 cyclopentadien-1-yl]-, 67-63-0 Me₂CHOH
 SOL 67-63-0 Me₂CHOH, 108-88-3 PhMe
 CON 20 hours, 70 deg C

REFERENCE COUNT: 109 THERE ARE 109 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L118 ANSWER 3 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 3
 ACCESSION NUMBER: 143:133122 CASREACT Full-text
 TITLE: Dynamic kinetic resolution of secondary alcohols by
 enzyme-metal combinations in ionic liquid
 AUTHOR(S): Kim, Mahn-Joo; Kim, Hyun Min; Kim,
 Daeho; Ahn, Yangsoo; Park, Jaiwook
 CORPORATE SOURCE: National Research Laboratory of Chirotechnology,
 Department of Chemistry, Division of Molecular and
 Life Sciences, Pohang University of Science and
 Technology, Pohang, 790-784, S. Korea
 SOURCE: Green Chemistry (2004), 6(9), 471-474
 CODEN: GRCHFJ; ISSN: 1463-9262
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Secondary aralkyl alcs. undergo enantioselective acylation in ionic liqs. in
 the presence of bis(cymenedichlororuthenium) and either lipase or subtilisin.
 In ionic liqs. such as [BMIM]⁺PF₆⁻ (BMIM⁺ = 1-butyl-3-methylimidazolium),
 bis(cymenedichlororuthenium) racemizes secondary alcs. such as (S)-1-
 phenylethanol efficiently; the ruthenium complex racemizes secondary alcs.
 less effectively in conventional solvents such as methylene chloride, toluene,
 or THF. Secondary alcs. undergo enantioselective acylation and dynamic
 kinetic resolution with 2,2,2-trifluoroethyl acetate in the presence of
 bis(cymenedichlororuthenium) and lipase in [BMIM]⁺PF₆⁻ to give the (R)-
 secondary acetates in 85-92% yields and in 99% ee. In the presence of
 bis(cymenedichlororuthenium) and subtilisin in [BMIM]⁺PF₆⁻, secondary alcs.
 undergo acylation with 2,2,2-trifluoroethyl butyrate to give the secondary
 butyrate esters in 78-92% yields and in 85-99% ee; dialcs. are acylated to
 diesters in 52-63% diastereoselectivities.

RX(1) OF 25 A + B ==> C



RX(1) RCT A 406-95-1, B 698-87-3
 RGT D 121-44-8 Et₃N
 PRO C 116907-36-9

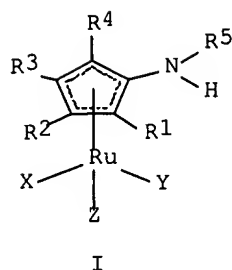
CAT 52462-29-0 Ruthenium, di- μ -
 chlorodichlorobis[(1,2,3,4,5,6- η)-1-methyl-4-(1-
 methylethyl)benzene]di-, 9001-62-1 Lipase
 SOL 174501-64-5 1H-Imidazolium, 1-butyl-3-methyl-,
 hexafluorophosphate(1-)
 CON 2 days, room temperature
 NTE **stereoselective**, enantioselective, biotransformation,
 enzymic, 99% ee

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 4 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 4
 ACCESSION NUMBER: 139:261424 CASREACT Full-text
 TITLE: Resolution of chiral compounds using
 aminocyclopentadienyl ruthenium catalysts
 INVENTOR(S): Park, Jaiwook; Kim, Mahn-joo;
 Choi, Jun Ho; Ahn, Yangsoo
 PATENT ASSIGNEE(S): Postech Foundation, S. Korea
 SOURCE: PCT Int. Appl., 21 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

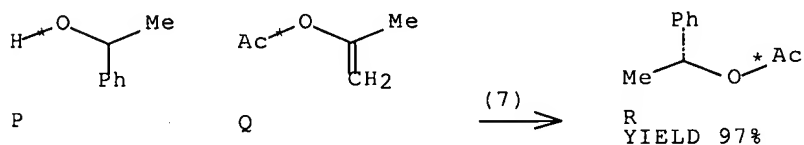
→ got d.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076384	A1	20030918	WO 2002-KR926	20020517
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2003074851	A	20030922	KR 2002-13832	20020314
CA 2478408	A1	20030918	CA 2002-2478408	20020517
AU 2002258278	A1	20030922	AU 2002-258278	20020517
EP 1483229	A1	20041208	EP 2002-728244	20020517
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1622932	A	20050601	CN 2002-828550	20020517
US 2005130282	A1	20050616	US 2004-507727	20040913
US 7156731	B2	20070102		
PRIORITY APPLN. INFO.:			KR 2002-13832	20020314
			WO 2002-KR926	20020517
OTHER SOURCE(S):			MARPAT 139:261424	
GI				



AB A chiral compound, particularly a chiral secondary alc., can be efficiently resolved under a mild condition by acylation with an alkenyl acetate in the presence of a novel aminocyclopentadienyl ruthenium complexes, I (preparation given; R1-R4 = (un)substituted Ph, C1-5 alkyl, etc.; R5 = H, (un)substituted Ph, C1-5 alkyl, C3-7 cycloalkyl, C2-5 alkenyl, C2-5 alkynyl, etc.; X, Y, Z = H, halo, CO, organophosphine), an enzyme catalyst, and a base. Thus, TiCl4-mediated reaction of tetraphenylcyclopentadienone with isobutylamine in PhMe gave N-isobutyl-2,3,4,5-tetraphenylcyclopentadieneimine which on treatment with Ru3(CO)12 gave title catalyst, N-isobutylamino-2,3,4,5-tetraphenylcyclopentadienylruthenium dicarbonyl chloride (II). . II catalyzed resolution of 1-phenylethanol in presence of Na2CO3/KOBu-t/Candida antarctica lipase B and isopropenyl acetate gave 97% (R)-1-phenylethyl acetate with 99% enantiomeric excess.

RX(7) OF 15 P + Q ==> R



RX(7) RCT P 98-85-1, Q 108-22-5
 RGT S 865-47-4 t-BuOK, M 497-19-8 Na2CO3
 PRO R 16197-92-5
 CAT 600136-35-4 Ruthenium, dicarbonylchloro[(1,2,3,4,5-
 η)-1-[(2-methylpropyl)amino]-2,3,4,5-tetraphenyl-2,4-
 cyclopentadien-1-yl]-
 SOL 108-88-3 PhMe
 CON 30 hours, room temperature
 NTE enzymic, stereoselective, Candida antatctica lipase B,
 biotransformation

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 5 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 5
 ACCESSION NUMBER: 139:337584 CASREACT Full-text
 TITLE: (S)-Selective Dynamic Kinetic Resolution of Secondary
 Alcohols by the Combination of Subtilisin and an

Aminocyclopentadienylruthenium Complex as the Catalysts

AUTHOR(S):

Kim, Mahn-Joo; Chung, Yong Il;
Choi, Yoon Kyung; Lee, Han Ki;
Kim, Daeho; Park, Jaiwook

CORPORATE SOURCE:

National Research Laboratory of Chirrotechnology,
Department of Chemistry, Division of Molecular and
Life Sciences, Pohang University of Science and
Technology, Kyongbuk, 790-784, S. Korea

SOURCE:

Journal of the American Chemical Society (2003),
125(38), 11494-11495

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

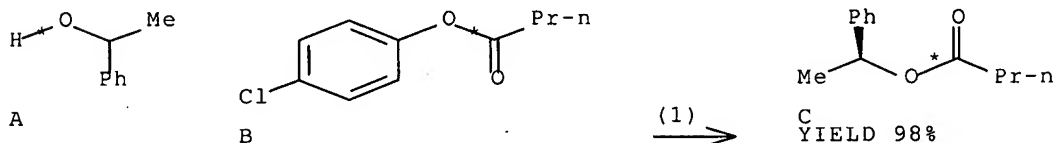
English

→ go + d.

AB A new procedure for the dynamic kinetic resolution (DKR) of racemic alcs. into single enantiomers is described. This procedure employs surfactant-treated subtilisin as an (S)-selective resolving catalyst and an aminocyclopentadienylruthenium complex as a racemizing catalyst. The DKR is performed best in the presence of an acyl donor such as trifluoroethyl butyrate in THF at room temperature. Eight simple secondary alcs. have been efficiently resolved with high optical purities and good yields. The subtilisin-based DKR is complementary in stereoselectivity to its lipase-based counterpart. For an acyl-carrying alc., both subtilisin- and lipase-based DKRs have proceeded equally well to give a pair of enantiomeric products (>99.5% ee each) with opposite optical rotations in high yields (94-95%).

RX(1) OF 13

A + B ==> C



RX(1)

STAGE(1)

RGT D 9004-95-9 Poly(oxy-1,2-ethanediyl), α -hexadecyl-
 ω -hydroxy-

CAT 9014-01-1 Subtilisin

SOL 110-86-1 Pyridine, 7732-18-5 Water

CON SUBSTAGE(1) 5 minutes, room temperature
SUBSTAGE(2) 12 hours, 35 deg C

STAGE(2)

RCT A 98-85-1, B 7476-81-5

RGT E 865-47-4 t-BuOK, F 497-19-8 Na₂CO₃CAT 470688-18-7 Ruthenium,
dicarbonylchloro[(1,2,3,4,5- η)-1-[(1-methylethyl)amino]-
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]-

SOL 109-99-9 THF

CON 3 days, 25 deg C

PRO C 161024-76-6

NTE optimization study, optimized on solvent,
stereoselective, stereoselectivity increased slightly
 with other acyl donor (TFEB), biotransformation, enzymic

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 6 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 137:311016 CASREACT Full-text

TITLE: Aminocyclopentadienyl ruthenium chloride: Catalytic
 racemization and dynamic kinetic resolution of
 alcohols at ambient temperature

AUTHOR(S): Choi, Jun Ho; Kim, Yu Hwan; Nam, Se Hyun;
 Shin, Seung Tae; Kim, Mahn-Joo; Park,
 Jaiwook

CORPORATE SOURCE: National Research Laboratory of Chirrotechnology
 Department of Chemistry Division of Molecular and Life
 Sciences, Pohang University of Science and Technology
 (POSTECH), Pohang, 790-784, S. Korea

SOURCE: Angewandte Chemie, International Edition (2002),
 41(13), 2373-2376

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

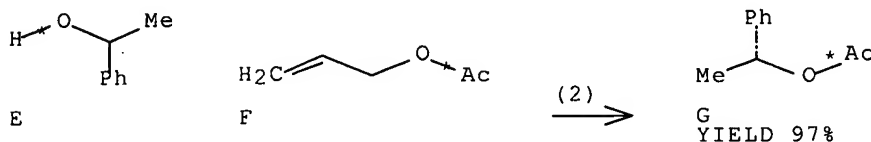
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Novel racemization catalyst is prepared, $[\text{RuCl}(\text{CO})_2(\eta^5\text{-cyclo-C}_5\text{Ph}_4\text{NHCHMe}_2)]$
 (1), which improves dramatically the ruthenium-enzyme tandem dynamic kinetic
 resolution (DKR) of secondary alcs. The DKR proceeds at room temperature with
 isopropenyl acetate as an acyl donor and requires less lipase than with
 racemization catalysts described earlier. The structure of 1 was determined
 by x-ray diffraction.

→ get it (good date)

RX(2) OF 12 E + F ==> G



RX(2) RCT E 98-85-1, F 591-87-7

RGT H 497-19-8 Na₂CO₃

PRO G 16197-92-5

CAT 470688-18-7 Ruthenium, dicarbonylchloro[(1,2,3,4,5-
 η)-1-[(1-methylethyl)amino]-2,3,4,5-tetraphenyl-2,4-
 cyclopentadien-1-yl]-, 865-47-4 t-BuOK, 9001-62-1 Lipase

SOL 108-88-3 PhMe

NTE **stereoselective**, >99% ee, enzymic, 25°, 30 h
 under argon

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

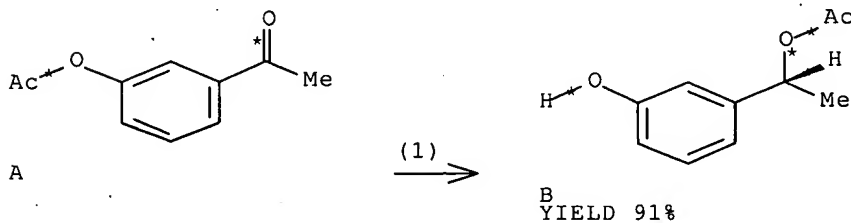
L118 ANSWER 7 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 140:405582 CASREACT Full-text
 TITLE: Method for the preparation of chiral hydroxy esters by
 enzyme/metal multi-catalysis
 INVENTOR(S): Kim, Mahn-joo; Park, Jai-wook;
 Han, Min-young; Choi, Min-young; Choi,
 Yoon-kyung; Lee, Jae-kwan
 PATENT ASSIGNEE(S): Postech Foundation, S. Korea
 SOURCE: PCT Int. Appl., 21 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

Ygt 3.
Good date

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039998	A1	20040513	WO 2003-KR1437	20030721
W: CA, CN, IN, JP, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
KR 2004038176	A	20040508	KR 2002-67058	20021031
PRIORITY APPLN. INFO.:			KR 2002-67058	20021031
OTHER SOURCE(S):			MARPAT 140:405582	

AB The invention provides a process for preparing a chiral hydroxy ester by reacting a compound having both a ketone group and an acyloxy group in a mol. with a hydrogen donor which reduces the ketone group into an hydroxyl group; a metal complex, which catalyzes both the reduction of the ketone and racemization reaction of produced hydroxy group; and an enzyme, which catalyzes enantioselective acyl transfer in an organic solvent.

RX(1) OF 8 A ==> B



RX(1) RCT A 2454-35-5

STAGE(1)

CAT 9001-62-1 Lipase, 104439-77-2 Ruthenium,
 tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-
 η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-
 yl]di-

SOL 108-88-3 PhMe
CON room temperature

STAGE(2)

RGT C 1333-74-0 H2
CON 72 hours, room temperature

PRO B 490031-20-4

NTE biotransformation, enzymic, stereoselective,
Pseudomonas cepacia lipase/Candida antarctica lipase/Candida
rugosa lipase used

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 8 OF 24 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 138:122426 CASREACT Full-text

TITLE: Asymmetric Transformations of Acyloxyphenyl Ketones by
Enzyme-Metal Multicatalysis

AUTHOR(S): Kim, Mahn-Joo; Choi, Min Young; Han, Min
Young; Choi, Yoon Kyung; Lee, Jae Kwan;
Park, Jaiwook

CORPORATE SOURCE: National Research Laboratory of Chirotechnology,
Department of Chemistry, Division of Molecular and
Life Sciences, Pohang University of Science and
Technology, Kyongbuk, 790-784, S. Korea

SOURCE: Journal of Organic Chemistry (2002), 67(26), 9481-9483
CODEN: JOCEAH; ISSN: 0022-3263

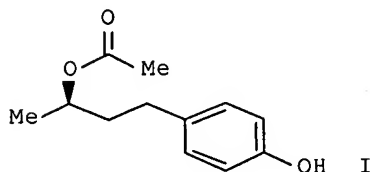
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

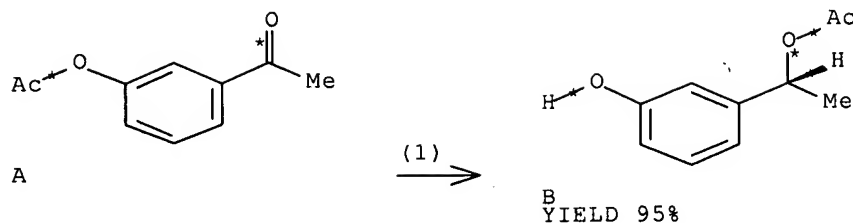
GI

y got d.



AB A multipathway process comprising several enzyme- and metal-catalyzed reactions has been explored for the asym. transformations of acyloxyphenyl ketones to optically active hydroxyphenyl alcs. in the ester forms, e.g., I. The process comprises nine component reactions in three pathways, all of which take place by the catalytic actions of only two catalysts, a lipase and a ruthenium complex. The synthetic reactions were carried out on 0.2-0.6 mmol scales for eight different substrates under an atmospheric of hydrogen (1 atm) in toluene at 70 °C for 3 days. In most cases, the yields were high (92-96%) and the optical purities were excellent (96-98% ee). This work thus has demonstrated that enzyme-metal multicatalysis has great potential as a new methodol. for asym. transformations.

RX(1) OF 8 A ==> B



RX(1) RCT A 2454-35-5
 RGT C 1333-74-0 H2
 PRO B 490031-20-4
 CAT 104439-77-2 Ruthenium, tetracarbonyl-μ-
 hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-
 cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-
 tetraphenyl-2,4-cyclopentadien-1-yl]di-, 9001-62-1 Lipase
 SOL 108-88-3 PhMe
 CON 3 days, 70 deg C
 NTE biotransformation, **stereoselective**, lipase PS-D used
 REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 9 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 134:310984 CASREACT Full-text
 TITLE: Preparation of chiral esters
 INVENTOR(S): Park, Jai Wook; Kim, Mahn-joo;
 Koh, Jeong Hwan; Jung, Hyun Min
 PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang
 University of Science and Technology
 SOURCE: PCT Int. Appl., 20 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001028971	A1	20010426	WO 2000-KR1171	20001018
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2387950	A1	20010426	CA 2000-2387950	20001018
AU 2001010589	A	20010430	AU 2001-10589	20001018
KR 2001040122	A	20010515	KR 2000-61351	20001018
EP 1226105	A1	20020731	EP 2000-971840	20001018

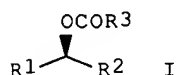
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL

JP 2003512035 T 20030402 JP 2001-531776 20001018

PRIORITY APPLN. INFO.: KR 1999-45041 19991018

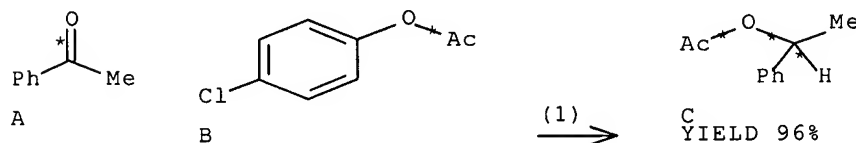
WO 2000-KR1171 20001018

OTHER SOURCE(S): MARPAT 134:310984
GI



AB Title esters [I; R1-R3 = (cyclo)alkyl, aryl, etc.] were prepared from R1COR2 in the presence of a Ru complex, a lipase, a hydride donor, and an acyl donor wherein unacylated alkanol enantiomer is racemized providing for complete conversion..

RX(1) OF 7 A + B ==> C



RX(1) RCT A 98-86-2

STAGE(1)

RGT D 121-44-8 Et3N, E 108-82-7 4-Heptanol, 2,6-dimethyl-, F
9001-62-1 Lipase

CAT 52462-29-0 Ruthenium, di-μ-
chlorodichlorobis[(1,2,3,4,5,6-η)-1-methyl-4-(1-
methylethyl)benzene]di-

SOL 75-09-2 CH2Cl2

STAGE(2)

RCT B 876-27-7

PRO C 93-92-5

NTE enzymic, biotransformation, **stereoselective**

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 10 OF 24 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 134:310983 CASREACT Full-text

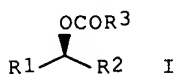
TITLE: Preparation of chiral esters

INVENTOR(S): Park, Jai Wook; Kim, Mahn-joo;

PATENT ASSIGNEE(S): Koh, Jeong Hwan; Jung, Hyun Min
 Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang
 University of Science and Technology
 SOURCE: PCT Int. Appl., 23 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

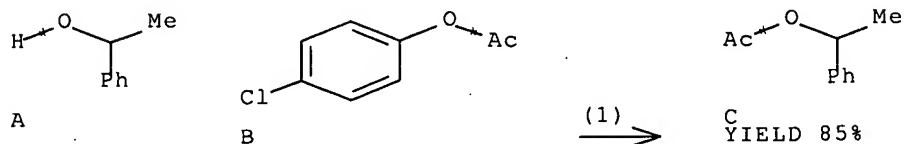
get d.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001028970	A1	20010426	WO 2000-KR1170	20001018
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2387949	A1	20010426	CA 2000-2387949	20001018
AU 2001010588	A	20010430	AU 2001-10588	20001018
KR 2001040121	A	20010515	KR 2000-61350	20001018
EP 1228033	A1	20020807	EP 2000-971839	20001018
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003512034	T	20030402	JP 2001-531775	20001018
US 6753443	B1	20040622	US 2001-786276	20010302
PRIORITY APPLN. INFO.:			KR 1999-45040	19991018
OTHER SOURCE(S):			WO 2000-KR1170	20001018
GI			MARPAT 134:310983	



AB Title esters [I; R1-R3 = (cyclo)alkyl, aryl, etc.] were prepared from racemic alkanols in the presence of a Ru complex, a lipase, and an acyl donor wherein unacylated alkanol enantiomer is racemized providing for complete conversion.

RX(1) OF 6 A + B ==> C

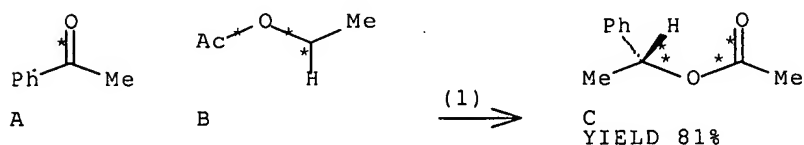


RX(1) RCT A 98-85-1, B 876-27-7
 RGT D 121-44-8 Et₃N
 PRO C 93-92-5
 CAT 99897-61-7 Ruthenium, chloro[(1,2,3,3a,7a-η)-1H-inden-1-yl]bis(triphenylphosphine)-
 SOL 75-09-2 CH₂Cl₂
 NTE STEREOSELECTIVE, LIPASE USED
 REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 11 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 133:237398 CASREACT Full-text
 TITLE: Practical Ruthenium/Lipase-Catalyzed Asymmetric Transformations of Ketones and Enol Acetates to Chiral Acetates
 AUTHOR(S): Jung, Hyun M.; Koh, Jeong H.; Kim, Mahn-Joo; Park, Jaiwook
 CORPORATE SOURCE: Department of Chemistry Division of Molecular Life Science, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, S. Korea
 SOURCE: Organic Letters (2000), 2(16), 2487-2490 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Ketones were asym. transformed to chiral acetates by one-pot processes using a lipase and an achiral ruthenium complex under 1 atm of hydrogen gas in Et acetate. Mol. hydrogen was also effective for the transformation of enol acetates to chiral acetates without addnl. acyl donors with the same catalyst system.

RX(1) OF 18 A + B ==> C



RX(1) RCT A 98-86-2, B 141-78-6

STAGE(1)

RGT D 9001-62-1 Lipase
 SOL 141-78-6 AcOEt

STAGE(2)

RGT E 1333-74-0 H₂
 CAT 104439-77-2 Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-

2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-

PRO C 16197-92-5
NTE STERESELECTIVEREFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 12 OF 24 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 132:222047 CASREACT Full-textTITLE: Concerted Catalytic Reactions for Conversion of
Ketones or Enol Acetates to Chiral AcetatesAUTHOR(S): Jung, Hyun M.; Koh, Jeong H.; Kim, Mahn-Joo;
Park, JaiwookCORPORATE SOURCE: Department of Chemistry and Division of Molecular &
Life Science, Pohang University of Science and
Technology (POSTECH), Pohang, 790-784, S. Korea

SOURCE: Organic Letters (2000), 2(3), 409-411

CODEN: ORLEF7; ISSN: 1523-7060

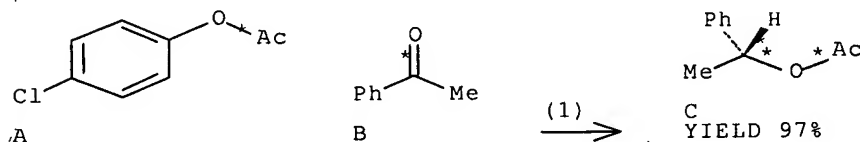
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Enol acetates or ketones asym. transformed to chiral acetates in high yields with high optical purities through multistep reactions catalyzed by a lipase and a ruthenium complex. 2,6-Dimethyl-4-heptanol was chosen as a suitable hydrogen donor, and 4-chlorophenyl acetate was used as an acyl donor for the conversion of ketones.

RX(1) OF 16 A + B ==> C



RX(1) RCT A 876-27-7, B 98-86-2

RGT D 9001-62-1 Lipase

PRO C 16197-92-5

CAT 104439-77-2 Ruthenium, tetracarbonyl-μ-
hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-
cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-
tetraphenyl-2,4-cyclopentadien-1-yl]di-

SOL 108-88-3 PhMe

NTE stereoselective, ultrasound to increase dispersion in
suspension, biotransformation, Novozym 435 usedREFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 13 OF 24 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 131:286217 CASREACT Full-text

TITLE: Enzymatic resolution of secondary alcohols coupled

with ruthenium-catalyzed racemization without hydrogen mediator

AUTHOR(S): Koh, Jeong Hwan; Jung, Hyun Min; Kim, Mahn-Joo; Park, Jaiwook

CORPORATE SOURCE: Department of Chemistry and Center for Biofunctional Molecules, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, S. Korea

SOURCE: Tetrahedron Letters (1999), 40(34), 6281-6284
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

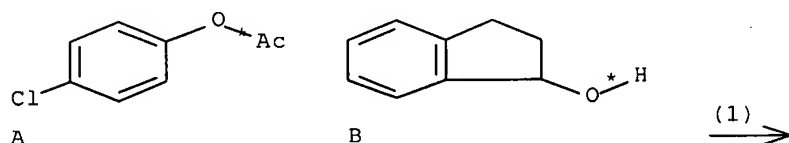
DOCUMENT TYPE: Journal

LANGUAGE: English

1 got 4.

AB (η^5 -Indenyl)RuCl(PPh₃)₂ was found to catalyze the racemization of secondary alcs. in the presence of triethylamine and oxygen. Unlike previously reported metal-catalyzed racemization, ketones were not required as hydrogen mediators in our process. The Ru-catalyzed racemization was coupled with enzymic acetylation for the dynamic kinetic resolution of secondary alcs. to give chiral acetates in good yields (60-98%) with high enantioselectivities (82-99% ee). For example, chloro(η^5 -indenyl)bis(triphenylphosphine)ruthenium-catalyzed racemization of (\pm)-1-phenylethanol coupled with lipase-catalyzed acetylation gave (R)-1-phenylethanol acetate in 85% yield (96% enantiomeric excess).

RX(1) OF 6 A + B ==> C

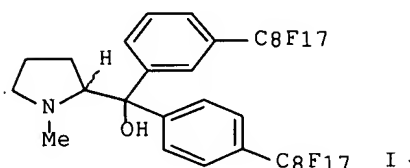


C
YIELD 88%

RX(1) RCT A 876-27-7, B 6351-10-6
 RGT D 121-44-8 Et₃N, E 7782-44-7 O₂
 PRO C 879-35-6
 CAT 9001-62-1 Lipase, 99897-61-7 Ruthenium,
 chloro[(1,2,3,3a,7a- η)-1H-inden-1-yl]bis(triphenylphosphine)-
 SOL 75-09-2 CH₂Cl₂
 CON 43 hours, 60 deg C
 NTE biotransformation, enzymic, stereoselective, ee 82%,
 Pseudomonas cepacia lipase enzyme used, dynamic kinetic
 resolution

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:101854 CAPLUS Full-text
 DOCUMENT NUMBER: 142:336082
 TITLE: Asymmetric diethyl- and diphenylzinc additions to aldehydes by using a fluorine-containing chiral amino alcohol: A striking temperature effect on the enantioselectivity, a minimal amino alcohol loading, and an efficient recycling of the amino alcohol
 AUTHOR(S): Park, Jin Kyoon; Lee, Hong Geun; Bolm, Carsten; Kim, B. Moon
 CORPORATE SOURCE: School of Chemistry, Seoul National University, Seoul, 151-747, S. Korea
 SOURCE: Chemistry--A European Journal (2005), 11(3), 945-950
 CODEN: CEUJED; ISSN: 0947-6539
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:336082
 ED Entered STN: 07 Feb 2005
 GI



- AB A chiral pyrrolidinylmethanol derivative containing perfluoro-ponytails I was prepared from (S)-proline. The use of this perfluoro-substituted amino alc. in catalytic asym. addns. of organozinc reagents to aldehydes affords products with high enantioselectivities in both pure hexane and a mixture of hexane and FC-72 (perfluorohexane). Enantiomeric excesses up to 94 and 88% ee have been achieved in Et₂Zn and Ph₂Zn addns., resp. For the reactions in the biphasic solvent system a striking temperature effect was observed. Thus, when the temperature was raised from 0 to 40°C the ee value of the product increased from 81 to 92%. Furthermore, the catalyst loading could be remarkably low, and with only 0.1 mol% of amino alc. 5 a product with 90% ee was obtained in the Et₂Zn addition to benzaldehyde in hexane. The perfluoro-ligand was easily recovered by simple phase separation, and until the ninth repetition its reuse proceeded without significant loss of enantioselectivity and reactivity.
- CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 34
- ST aryl aldehyde diorganozinc asym addn reaction fluorous amino alc
 ; chiral fluorous amino alc asym addn catalyst; benzyl
 alc stereoselective prepn
- IT Aldehydes, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aromatic; stereoselective preparation of benzylic alcs. via fluorous
 chiral amino alc. catalyzed asym. addition reaction of

- diorganozincs with arylaldehydes)
- IT Alcohols, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (benzyl, chiral; stereoselective preparation of benzylic
 alcs. via fluorous chiral amino alc.
 catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
- IT Alcohols, preparation
 RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation);
 PREP (Preparation); USES (Uses)
 (chiral, amino, fluorous; stereoselective preparation of benzylic
 alcs. via fluorous chiral amino alc.
 catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
- IT Partition
 (fluorous; partition coefficient evaluation and stereoselective preparation
 of
 benzylic alcs. via fluorous chiral amino
 alc. catalyzed asym. addition reaction of diorganozincs with
 arylaldehydes)
- IT Asymmetric synthesis and induction
 (stereoselective preparation of benzylic alcs. via fluorous
 chiral amino alc. catalyzed asym. addition reaction of
 diorganozincs with arylaldehydes)
- IT Addition reaction
 Addition reaction catalysts
 (stereoselective; stereoselective preparation of benzylic alcs.
 via fluorous chiral amino alc. catalyzed asym.
 addition reaction of diorganozincs with arylaldehydes)
- IT 848784-93-0P
 RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation);
 PREP (Preparation); USES (Uses)
 (partition coefficient; partition coefficient evaluation and
 stereoselective
 preparation of benzylic alcs. via fluorous chiral amino
 alc. catalyzed asym. addition reaction of diorganozincs with
 arylaldehydes)
- IT 110529-22-1
 RL: CAT (Catalyst use); USES (Uses)
 (stereoselective preparation of benzylic alcs. via fluorous
 chiral amino alc. catalyzed asym. addition reaction of
 diorganozincs with arylaldehydes)
- IT 100-52-7, Benzaldehyde, reactions 104-55-2, Cinnamaldehyde 104-88-1,
 p-Chlorobenzaldehyde, reactions 106-37-6, 1,4-Dibromobenzene 123-11-5,
 p-Methoxybenzaldehyde, reactions 507-63-1, Perfluorooctyl iodide
 557-20-0, Diethylzinc 1078-58-6, Diphenylzinc 93423-88-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (stereoselective preparation of benzylic alcs. via fluorous
 chiral amino alc. catalyzed asym. addition reaction of
 diorganozincs with arylaldehydes)
- IT 848784-90-7P 848784-91-8P 848784-92-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (stereoselective preparation of benzylic alcs. via fluorous
 chiral amino alc. catalyzed asym. addition reaction of
 diorganozincs with arylaldehydes)
- IT 613-87-6P 73854-04-3P 73890-73-0P 88765-29-1P 101402-04-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (stereoselective preparation of benzylic alcs. via fluorous
 chiral amino alc. catalyzed asym. addition reaction of
 diorganozincs with arylaldehydes)

REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:452908 CAPLUS Full-text

DOCUMENT NUMBER: 143:171348

TITLE: Dynamic kinetic resolutions and asymmetric transformations by enzyme-metal combo catalysis

AUTHOR(S): Kim, Mahn-Joo; Ahn, Yangsoo; Park, Jaiwook

CORPORATE SOURCE: National Research Laboratory of Chirotechnology and Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Kyongbuk, 790-784, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (2005), 26(4), 515-522

CODEN: BKCSDE; ISSN: 0253-2964

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

ED Entered STN: 27 May 2005

AB A review. Enzyme-metal combo catalysis is described as a useful methodol. for the synthesis of optically active compds. The key point of the method is the use of enzyme and metal in combination as the catalysts for the complete transformation of racemic substrates to single enantiomeric products through dynamic kinetic resolution (DKR). In this approach, enzyme acts as an enantioselective resolving catalyst and metal does as a racemizing catalyst for the efficient DKR. Three kinds of enzyme-metal combinations - lipase-ruthenium, subtilisin-ruthenium, and lipase-palladium - have been developed as the catalysts for the DKRs of racemic alcs., esters, and amines. The scope of the combination catalysts can be extended to the asym. transformations of ketones, enol acetates, and ketoximes via the DKRs. In most cases studied, enzyme-metal combo catalysis provided enantiomerically-enriched products in high yields.

CC 16-0 (Fermentation and Bioindustrial Chemistry)

IT Resolution (separation)

(enzymic; dynamic kinetic resolns. and asym.

transformations by enzyme-metal combo catalysis)

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:236729 CAPLUS Full-text

DOCUMENT NUMBER: 140:433486

TITLE: Fluorometric assay protocol for protease-catalyzed transesterification reactions in organic solvents

AUTHOR(S): Han, Min Su; Jung, Sang Oh; Kim, Mahn-Joo; Kim, Dong H.

CORPORATE SOURCE: Center for Integrated Molecular Systems, and National Research Laboratory of Chirotechnology, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Journal of Organic Chemistry (2004), 69(8), 2853-2855

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 23 Mar 2004

AB A fluorometric assay protocol for a subtilisin-catalyzed transesterification reaction in hexane has been developed. The method makes use of a Michael

acceptor that forms a fluorescent adduct with thiophenol, one of the products generated in the transesterification reaction. The method may be employed for screening a biocatalyst useful for transesterification reactions in organic solvents and for optimizing the transesterification reaction conditions. Thus, this protocol takes advantage of the facile Michael acceptor properties of a com. available dye, 7-diethylamino-3-(4'-maleimidylphenyl)-4-methylcoumarin, with benzenethiol formed in the above transesterification, thus giving a highly fluorescent product.

CC 80-5 (Organic Analytical Chemistry)

Section cross-reference(s): 25

IT Fluorescent substances

Michael reaction

Transesterification

(fluorometric assay protocol for protease-catalyzed transesterification of chiral (carbonylamino)benzenepropanethioic acid esters with alcs. and capture of benzenethiol with (diethylamino) (maleimidylphenyl) (methyl) coumarin)

IT Alcohols, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorometric assay protocol for protease-catalyzed transesterification of chiral (carbonylamino)benzenepropanethioic acid esters with alcs. and capture of benzenethiol with (diethylamino) (maleimidylphenyl) (methyl) coumarin)

IT 9014-01-1, Subtilisin

RL: CAT (Catalyst use); USES (Uses)

(Carlsberg; fluorometric assay protocol for protease-catalyzed transesterification of chiral (carbonylamino)benzenepropanethioic acid esters with alcs. and capture of benzenethiol with (diethylamino) (maleimidylphenyl) (methyl) coumarin)

IT 691413-66-8P

RL: BPN (Biosynthetic preparation); PNU (Preparation, unclassified); BIOL (Biological study); PREP (Preparation)

(fluorometric assay protocol for protease-catalyzed transesterification of chiral (carbonylamino)benzenepropanethioic acid esters with alcs. and capture of benzenethiol with (diethylamino) (maleimidylphenyl) (methyl) coumarin)

IT 108-98-5P, Benzenethiol, reactions

RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(fluorometric assay protocol for protease-catalyzed transesterification of chiral (carbonylamino)benzenepropanethioic acid esters with alcs. and capture of benzenethiol with (diethylamino) (maleimidylphenyl) (methyl) coumarin)

IT 9004-07-3, α -Chymotrypsin 37259-58-8, Serine protease

RL: CAT (Catalyst use); USES (Uses)

(fluorometric assay protocol for protease-catalyzed transesterification of chiral (carbonylamino)benzenepropanethioic acid esters with alcs. and capture of benzenethiol with (diethylamino) (maleimidylphenyl) (methyl) coumarin)

IT 71-23-8, 1-Propanol, reactions 811-51-8, Ethanethiol sodium salt

1161-13-3 2018-61-3 76877-33-3, 7-(Diethylamino)-3-(4'-maleimidylphenyl)-4-methylcoumarin

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorometric assay protocol for protease-catalyzed transesterification of chiral (carbonylamino)benzenepropanethioic acid esters with alcs. and capture of benzenethiol with (diethylamino) (maleimidylphenyl) (methyl) coumarin)

IT 2075-55-0P, (α S)- α -[[(Phenylmethoxy)carbonyl]amino]benzeneprop

anethioic acid S-phenyl ester 60718-38-9P, (α S)- α -

[[(Phenylmethoxy) carbonyl] amino] benzenepropanethioic acid S-ethyl ester
 79128-07-7P, (α S)- α -(Acetylamino)benzenepropanethioic acid
 S-phenyl ester 99685-32-2P, (α S)- α -
 (Acetylamino)benzenepropanethioic acid S-ethyl ester
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(fluorometric assay protocol for protease-catalyzed transesterification
 of chiral (carbonylamino)benzenepropanethioic acid esters
 with alcs. and capture of benzenethiol with
 (diethylamino) (maleimidylphenyl) (methyl) coumarin)

IT 110-54-3, Hexane, uses

RL: NUU (Other use, unclassified); USES (Uses)
 (fluorometric assay protocol for protease-catalyzed transesterification
 of chiral (carbonylamino)benzenepropanethioic acid esters
 with alcs. in organic solvents and capture of benzenethiol with
 (diethylamino) (maleimidylphenyl) (methyl) coumarin)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:96174 CAPLUS Full-text

DOCUMENT NUMBER: 140:4084

TITLE: Dynamic kinetic resolutions and asymmetric
 transformations by enzymes coupled with metal
 catalysis. [Erratum to document cited in CA138:186421]

AUTHOR(S): Kim, Mahn-Joo; Ahn, Yangsoo; Park,
 Jaiwook

CORPORATE SOURCE: Division of Molecular and Life Sciences, Department of
 Chemistry, National Research Laboratory of
 Chirotechnology, Pohang University of Science and
 Technology, Kyungbuk, 790-784, S. Korea

SOURCE: Current Opinion in Biotechnology (2003), 14(1), 131
 CODEN: CUOBE3; ISSN: 0958-1669

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

ED Entered STN: 07 Feb 2003

AB A review. The wrong legend was incorporated with Figure 6; the corrected
 version of the figure and legend is given. In the section on "Asym. reductive
 acetylation of ketoximes" the correct definition of Pd/C should have been
 given as palladium on carbon.

CC 16-0 (Fermentation and Bioindustrial Chemistry)

Section cross-reference(s): 7, 21

IT Resolution (separation)

(enzymic, kinetic; dynamic kinetic
 resolsns. and asym. transformations by enzymes coupled with metal
 catalysis (Erratum))

L118 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:931631 CAPLUS Full-text

DOCUMENT NUMBER: 138:186421

TITLE: Dynamic kinetic resolutions and asymmetric
 transformations by enzymes coupled with metal
 catalysis

AUTHOR(S): Kim, Mahn-Joo; Ahn, Yangsoo; Park,
 Jaiwook

CORPORATE SOURCE: Division of Molecular and Life Sciences, Department of
 Chemistry, National Research Laboratory of
 Chirotechnology, Pohang University of Science and
 Technology, Kyungbuk, 790-784, S. Korea

got it.

SOURCE: Current Opinion in Biotechnology (2002), 13(6),
578-587
CODEN: CUOBE3; ISSN: 0958-1669
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 09 Dec 2002
AB A review, with refs. The combination of enzyme and metal catalysis is described as a useful method for the synthesis of optically active compds. A key feature of this new methodol. is the use of metal catalysts for the in situ racemization of enzymically unreactive enantiomers in the enzymic resolution of racemic substrates. So far, two combinations - lipase-ruthenium and lipase-palladium - have been developed for the efficient dynamic kinetic resolution of alcs. and amines. The use of these combinations has also been extended to catalysis of the asym. transformation of ketones, their enol acetates, and ketoximes. In most cases, enzyme-metal combination catalysis has provided good yields and high optical purities. Coupled enzyme-metal catalysis is a new approach for the dynamic kinetic resolution and asym. transformations and provides a useful alternative to conventional chemical or enzymic methods.
CC 16-0 (Fermentation and Bioindustrial Chemistry)
Section cross-reference(s): 7, 21
IT Resolution (separation)
(enzymic, kinetic; dynamic kinetic
resolns. and asym. transformations by enzymes coupled with metal
catalysis)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:416874 CAPLUS Full-text
DOCUMENT NUMBER: 135:19231
TITLE: Stereoselective method for preparing chiral esters
from alkenyl esters via ruthenium catalyzed reduction
and enzymic resolution
INVENTOR(S): Park, Jai Wook; Kim, Mahn-joo;
Koh, Jeong Hwan; Jung, Hyun Min
PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang
University of Science and Technology
SOURCE: PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001040157	A1	20010607	WO 2000-KR1169	20001018
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2393336	A1	20010607	CA 2000-2393336	20001018
AU 2001010587	A5	20010612	AU 2001-10587	20001018
KR 2001060160	A	20010706	KR 2000-61352	20001018

EP 1237837	A1	20020911	EP 2000-971838	20001018
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003515336	T	20030507	JP 2001-541847	20001018
US 2001012898	A1	20010809	US 2000-726412	20001201
US 6475773	B2	20021105		

) got ch.

PRIORITY APPLN. INFO.:

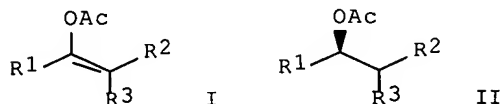
KR 1999-54472 A 19991202

WO 2000-KR1169 W 20001018

OTHER SOURCE(S): CASREACT 135:19231; MARPAT 135:19231

ED Entered STN: 08 Jun 2001

GI



- AB A method for preparing optically pure chiral esters I (R1, R2 and R3 = independently (un)substituted alkyl, aryl or cycloalkyl group and R1 and R2, R1 and R3, and R2 and R3 can form a cyclic ring; substituent may be halogen or cyano group) in high yield from alkenyl esters via ruthenium catalyzed reduction/racemization with successive enzymic resolution is disclosed. For example, II was synthesized in 89% yield (98% enantiomeric excess) by mixing 1-phenylethenyl acetate with 2,6-dimethylheptan-4-ol, a ruthenium catalyst, and Novozym 435 followed by heating under Argon with subsequent chromatog. purification. The chiral esters obtained can be used as synthetic intermediates for preparing various chiral compds., chiral pharmaceutical drugs (e.g. Atorvastatin and Agenerase) or chiral agrochems. (e.g. L-Carnitine).
- IC ICM C07C051-16
ICS C12P007-00
- CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 29
- IT Esters, preparation
RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation)
(chiral; stereoselective method for preparing chiral esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic alc. intermediate)
- IT Resolution (separation)
(enzymic, kinetic; stereoselective method for preparing chiral esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic alc. intermediate)
- IT Burkholderia cepacia
Candida antarctica
(lipase from; stereoselective method for preparing chiral esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic alc. intermediate)
- IT Hydrogenation
Stereoselective synthesis
(stereoselective method for preparing chiral esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic alc. intermediate)
- IT 54712-18-4P 58396-29-5P 68567-23-7P 115729-61-8P 129098-41-5P
137408-28-7P 137408-29-8P

RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation) (stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc.** intermediate)

IT 9001-62-1, Novozym 435 52462-29-0 104439-77-2

RL: CAT (Catalyst use); USES (Uses) (stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc.** intermediate)

IT 16197-93-6P

RL: IMF (Industrial manufacture); PREP (Preparation) (stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc.** intermediate)

IT 2206-94-2, 1-Phenylethenyl acetate 19455-83-5 22390-98-3 22479-32-9
26735-85-3 52789-67-0 260980-77-6 342808-62-2

RL: RCT (Reactant); RACT (Reactant or reagent) (stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc.** intermediate)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:877563 CAPLUS Full-text

DOCUMENT NUMBER: 142:74253

TITLE: Process for preparation of **chiral** allyl alcohol

INVENTOR(S): Choi, Yun Gyeong; Huh, Eun A.; Jung, Jae Yun; Kim, Man Ju; Lee, Dong Hyeon; Seo, Jong Hwa

PATENT ASSIGNEE(S): Postech Foundation, S. Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given
CODEN: KRXXA7

DOCUMENT TYPE: Patent

LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
KR 2001037656	A	20010515	KR 1999-45308	19991019
PRIORITY APPLN. INFO.:			KR 1999-45308	19991019

ED Entered STN: 22 Oct 2004

AB Provided is a process for producing **chiral** allyl **alc.** excellent in optical purity and synthetic yield by using a palladium metal catalyst for racemization of **chiral** allyl ester and an enzyme for producing the **chiral** allyl **alc.** from the racemic allyl ester. The **chiral** allyl **alc.** is produced by reacting the allyl ester, more than 5 mol% (based on the allyl ester) of the palladium(0) complex for the racemization of the allyl ester, 0.2-0.8 g (based on the racemic allyl ester of 1 mmol) of lipase for diacylating selectively an enantiomer of the allyl ester, and more than 10 equiv (based on the racemic allyl ester) of an acyl acceptor. The palladium(0) complex is selected from the group consisting of Pd(PPh₃)₄ and tris(dibenzylidene acetone)dipalladium(0). The acyl acceptor is selected from the group consisting of iso-Pr **alc.**, Pr **alc.**, Bu **alc.**, and pentyl **alc.**

IC ICM C07C029-00

CC 23-7 (Aliphatic Compounds)

ST **chiral** allyl **alc** prepn palladium catalytic

racemization
 IT 107-18-6P, Allyl alcohol, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of chiral allyl alc.)

L118 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:412568 CAPLUS Full-text
 DOCUMENT NUMBER: 135:152357
 TITLE: Lipase/Ruthenium-Catalyzed Dynamic Kinetic Resolution
 of Hydroxy Acids, Diols, and Hydroxy Aldehydes
 Protected with a Bulky Group
 AUTHOR(S): Kim, Mahn-Joo; Choi, Yoon Kyung;
 Choi, Min Young; Kim, Mi Jung; Park,
 Jaiwook
 CORPORATE SOURCE: National Research Laboratory of Chirotechnology
 Department of Chemistry Division of Molecular and Life
 Sciences, Pohang University of Science and Technology,
 Pohang Kyungbuk, 790-784, S. Korea
 SOURCE: Journal of Organic Chemistry (2001), 66(13), 4736-4738
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:152357
 ED Entered STN: 08 Jun 2001
 AB The racemic title substrates were modified with bulky protecting groups and
 then subjected to the lipase/ruthenium-catalyzed dynamic kinetic resolution
 (DKR). E.g., DKR of MeCH(OH)CH₂CO₂CH₂Ph with Pseudomonas cepacia lipase, a Ru
 catalyst, and 4-ClC₆H₄OAc gave (R)-MeCH(OAc)CH₂CO₂CH₂Ph (88% yield, 86 % ee).
 CC 21-2 (General Organic Chemistry)
 IT Resolution (separation)
 (kinetic; lipase/ruthenium-catalyzed dynamic
 kinetic resolution of hydroxy acids, diols, and hydroxy aldehydes
 protected with a bulky group)
 REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:455856 CAPLUS Full-text
 DOCUMENT NUMBER: 133:222192
 TITLE: Dynamic Kinetic Resolution of Allylic Alcohols
 Mediated by Ruthenium- and Lipase-Based Catalysts
 AUTHOR(S): Lee, Donghyun; Huh, Eun A.; Kim, Mahn-Joo;
 Jung, Hyun Min; Koh, Jeong Hwan; Park, Jaiwook
 CORPORATE SOURCE: Department of Chemistry Division of Molecular and Life
 Science, Pohang University of Science and Technology,
 Pohang Kyungbuk, 790-784, S. Korea
 SOURCE: Organic Letters (2000), 2(15), 2377-2379
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 133:222192
 ED Entered STN: 07 Jul 2000
 AB An enzyme-metal combo reaction has been developed for the dynamic kinetic
 resolution of allylic alcs. in which racemic substrates are transformed by a
 lipase and a ruthenium complex in the presence of an acyl donor to allylic
 acetates of high optical purity in over 80% yield.
 CC 21-3 (General Organic Chemistry)
 Section cross-reference(s): 16

IT Racemization
 Racemization
 (catalysts, Ru-catalyzed racemization of **chiral allylic alcs.**; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic alcs. and Ru-catalyzed racemization of unreacted substrate)

IT Racemization
 (of **chiral allylic alcs.**; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic alcs. and Ru-catalyzed racemization of unreacted substrate)

IT Isomerization catalysts
 Isomerization catalysts
 (racemization catalysts, Ru-catalyzed racemization of **chiral allylic alcs.**; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic alcs. and Ru-catalyzed racemization of unreacted substrate)

IT 122-57-6P, 3-Buten-2-one, 4-phenyl- 2550-26-7P, Butan-2-one, 4-phenyl-
 RL: BYP (Byproduct); PREP (Preparation)
 (side-product in racemization of **chiral allylic alcs** .; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic alcs. and Ru-catalyzed racemization of unreacted substrate)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:643342 CAPLUS Full-text

DOCUMENT NUMBER: 132:35316

TITLE: Dynamic Kinetic Resolution of Acyclic Allylic Acetates Using Lipase and Palladium

AUTHOR(S): Choi, Yoon Kyung; Suh, Jong Hwa; Lee, Donghyun; Lim, In Taek; Jung, Jae Yoon; Kim, Mahn-Joo

CORPORATE SOURCE: Department of Chemistry and Center for Biofunctional Molecules, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Journal of Organic Chemistry (1999), 64(22), 8423-8424
 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:35316

ED Entered STN: 11 Oct 1999

AB Racemic allylic acetates MeCH(OAc)CH:CHR (R = Ph, 4-ClC₆H₄, 4-MeC₆H₄, 2-furyl, 1-naphthyl) were transformed into single enantiomeric products (R)-MeCH(OH)CH:CHR through lipase-catalyzed transesterification coupled with Pd-catalyzed racemization.

CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 7, 9

IT Resolution (separation)

(kinetic; dynamic kinetic resolution of acyclic allylic acetates through lipase-catalyzed transesterification coupled with Pd-catalyzed racemization)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:101619 CAPLUS Full-text

DOCUMENT NUMBER: 128:200296

TITLE: Enantioselectivity of heptakis(6-O-alkyldimethylsilyl-2,3-di-O-ethyl)- β -cyclodextrins as chiral stationary phases in capillary gas chromatography

AUTHOR(S): Kim, Byoung Eog; Kim, Min Kyun; Ryu, Young Kyun; Park, Jung Kon; Park, Jung Hag

CORPORATE SOURCE: Research Institute of Industrial Science and Technology, Pohang, 790-330, S. Korea

SOURCE: Analytical Sciences (1997), 13(Suppl., Asianalysis IV), 263-266
CODEN: ANSCEN; ISSN: 0910-6340

PUBLISHER: Japan Society for Analytical Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 20 Feb 1998

AB Four heptakis(6-O-alkyldimethylsilyl-2,3-di-O-ethyl)- β -cyclodextrin (CD) having 6-O-alkyl groups of different chain length, heptakis(6-O-trimethylsilyl-2,3-di-O-ethyl)- β -CD (MTDE- β -CD), heptakis(6-O-ethyldimethylsilyl-2,3-di-O-ethyl)- β -CD (ETDE- β -CD), heptakis(6-O-octyldimethylsilyl-2,3-di-O-ethyl)- β -CD (OTDE- β -CD) and heptakis(6-O-octadecyldimethylsilyl-2,3-di-O-ethyl)- β -CD (ODDE- β -CD), were prepared and effect of the chain length of the 6-O-alkyl moiety on the enantioselectivity of the CD derivs. as chiral stationary phases were compared by measuring separation factors of a range of chiral test compds. in capillary gas chromatog. Enantioselectivity of the CD derivs. is in the order, ETDE- β -CD \geq MTDE- β -CD > OTDE- β -CD > ODDE- β -CD.

CC 80-4 (Organic Analytical Chemistry)

IT 78-76-2, (\pm)-2-Bromobutane 80-56-8, (\pm)- α -Pinene 93-54-9, (\pm)-1-Phenyl-1-propanol 98-85-1, (\pm)-sec-Phenethyl alcohol 107-81-3, (\pm)-2-Bromopentane 120-45-6, (\pm)-1-Phenylethyl propionate 138-86-3, (\pm)-Limonene 598-32-3, (\pm)-3-Buten-2-ol 613-87-6, (-)-1-Phenyl-1-propanol 822-67-3, (\pm)-2-Cyclohexen-1-ol 926-58-9, (-)-trans-3-Penten-2-ol 1072-86-2, (-)-trans-1,2-Cyclohexanediol 1123-85-9, (\pm)-2-Phenyl-1-propanol 1445-91-6, (-)-sec-Phenethyl alcohol 1460-57-7, (\pm)-trans-1,2-Cyclohexanediol 1517-69-7, (+)-sec-Phenethyl alcohol 1565-74-8, (+)-1-Phenyl-1-propanol 1974-04-5, (\pm)-2-Bromoheptane 2902-96-7, (\pm)-2-Nitro-1-propanol 3413-44-3, (+)-2-Cyclohexen-1-ol 3899-34-1, (\pm)-trans-3-Penten-2-ol 5787-32-6, (+)-2-Bromobutane 5787-33-7, (-)-2-Bromobutane 5989-27-5, (+)-Limonene 5989-54-8, (-)-Limonene 6118-13-4, (+)-3-Buten-2-ol 6426-26-2, (-)-2-Cyclohexen-1-ol 7785-26-4, (-)- α -Pinene 7785-70-8, (+)- α -Pinene 19141-40-3, (+)-2-Phenyl-1-propanol 29117-44-0, (-)-2-Bromopentane 29882-58-4, (+)-2-Bromopentane 33447-72-2, (-)-3-Buten-2-ol 35666-69-4, (+)-trans-3-Penten-2-ol 37778-99-7, (-)-2-Phenyl-1-propanol 57794-08-8, (+)-trans-1,2-Cyclohexanediol 107832-32-6, (R)-1-Phenylethyl propionate 117290-46-7, (S)-1-Phenylethyl propionate 130232-91-6, (+)-2-Bromoheptane 130232-92-7, (-)-2-Bromoheptane 192045-60-6, (R)-2-Nitro-1-propanol 192045-61-7, (S)-2-Nitro-1-propanol

RL: ANT (Analyte); PEP (Physical, engineering or chemical process); PRP (Properties); ANST (Analytical study); PROC (Process)
(enantioselectivity of heptakis(6-O-alkyldimethylsilyl-2,3-di-O-ethyl)- β -cyclodextrins as chiral stationary phases in capillary GC resolution of)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

REACTION SEARCH

=> fil casrea; d stat que 1125

FILE 'CASREACT' ENTERED AT 16:45:47 ON 02 FEB 2007

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 28 Jan 2007 VOL 146 ISS 5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 10 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
L14      152839 SEA FILE=REGISTRY ABB=ON RU/ELS
L24      1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
L25      1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
L67      72677 SEA FILE=CASREACT ABB=ON STEREOSELECTIVE/NTE
L68      30236 SEA FILE=REGISTRY ABB=ON L14 AND CASREACT/LC
L69      8227 SEA FILE=CASREACT ABB=ON L68/CAT
L70      267 SEA FILE=CASREACT ABB=ON L24/CAT OR L25/CAT
L73      76833 SEA FILE=CASREACT ABB=ON (L69 OR L70 OR L67)
L76      STR
```



NODE ATTRIBUTES:

```
CONNECT IS E3 RC AT 2
CONNECT IS E1 RC AT 4
CONNECT IS E3 RC AT 6
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 1
GGCAT IS UNS AT 5
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

```
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8
```

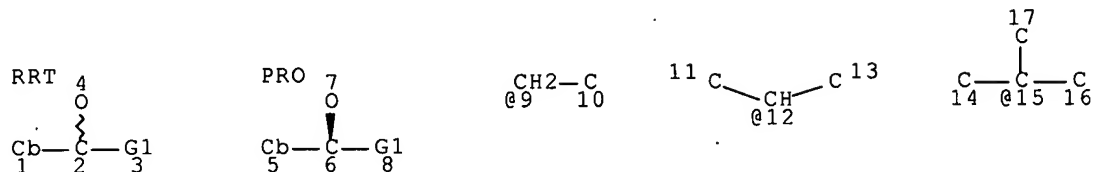
STEREO ATTRIBUTES:

STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1

****MAPPINGS****

NOD	SYM	ROL	NOD	SYM	ROL
2	C	RRT	6	C	PRO
4	O	RRT	7	O	PRO
6	C	PRO	2	C	RRT
7	O	PRO	4	O	RRT

L82 SCR 1149
L87 3195 SEA FILE=CASREACT SUB=L73 SSS FUL L76 AND L82 (20816 REACTIONS)
L122 STR



VAR G1=CH3/9/12/15

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 2
CONNECT IS E1 RC AT 4
CONNECT IS E3 RC AT 6
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 1
GGCAT IS UNS AT 5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES:

STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1

****MAPPINGS****

NOD	SYM	ROL	NOD	SYM	ROL
2	C	RRT	6	C	PRO
4	O	RRT	7	O	PRO
6	C	PRO	2	C	RRT
7	O	PRO	4	O	RRT

L124 1785 SEA FILE=CASREACT SUB=L87 SSS FUL L122 (10785 REACTIONS)
L125 1783 SEA FILE=CASREACT ABB=ON L124/COMPLETE

=> d que nos 1129; d que nos 1130; s 1129,1130 not 197

L14 152839 SEA FILE=REGISTRY ABB=ON RU/ELS
L24 1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
L25 1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
L67 72677 SEA FILE=CASREACT ABB=ON STEREOSELECTIVE/NTE
L68 30236 SEA FILE=REGISTRY ABB=ON L14 AND CASREACT/LC
L69 8227 SEA FILE=CASREACT ABB=ON L68/CAT
L70 267 SEA FILE=CASREACT ABB=ON L24/CAT OR L25/CAT
L73 76833 SEA FILE=CASREACT ABB=ON (L69 OR L70 OR L67)

L76 STR
 L82 SCR 1149
 L87 3195 SEA FILE=CASREACT SUB=L73 SSS FUL L76 AND L82 (20816 REACTIONS)
 L122 STR
 L124 1785 SEA FILE=CASREACT SUB=L87 SSS FUL L122 (10785 REACTIONS)
 L125 1783 SEA FILE=CASREACT ABB=ON L124/COMPLETE
 L129 9 SEA FILE=CASREACT ABB=ON L125(L)L70

L14 152839 SEA FILE=REGISTRY ABB=ON RU/ELS
 L24 1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
 L25 1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
 L67 72677 SEA FILE=CASREACT ABB=ON STEREOSELECTIVE/NTE
 L68 30236 SEA FILE=REGISTRY ABB=ON L14 AND CASREACT/LC
 L69 8227 SEA FILE=CASREACT ABB=ON L68/CAT
 L70 267 SEA FILE=CASREACT ABB=ON L24/CAT OR L25/CAT
 L73 76833 SEA FILE=CASREACT ABB=ON (L69 OR L70 OR L67)
 L76 STR
 L82 SCR 1149
 L87 3195 SEA FILE=CASREACT SUB=L73 SSS FUL L76 AND L82 (20816 REACTIONS)
 L104 9228 SEA FILE=CASREACT ABB=ON ENZYM?/NTE
 L122 STR
 L124 1785 SEA FILE=CASREACT SUB=L87 SSS FUL L122 (10785 REACTIONS)
 L125 1783 SEA FILE=CASREACT ABB=ON L124/COMPLETE
 L130 21 SEA FILE=CASREACT ABB=ON L125(L)L69(L)L67(L)L104

L131 17 (L129 OR L130) NOT L97

=> fil capl; d que l31; d que l30; d que l39; d que l42; d que l45
 FILE 'CAPLUS' ENTERED AT 16:46:32 ON 02 FEB 2007
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 2 Feb 2007 VOL 146 ISS 7
 FILE LAST UPDATED: 1 Feb 2007 (20070201/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>
 'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

L14 152839 SEA FILE=REGISTRY ABB=ON RU/ELS
 L15 101120 SEA FILE=CAPLUS ABB=ON L14
 L16 25439 SEA FILE=CAPLUS ABB=ON L15(L) CAT/RL
 L17 150091 SEA FILE=CAPLUS ABB=ON ALCOHOLS/CT
 L19 18354 SEA FILE=CAPLUS ABB=ON L17(L) PREP/RL
 L20 136 SEA FILE=CAPLUS ABB=ON L19(L) "S"/OBI
 L24 1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
 L25 1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
 L26 51371 SEA FILE=CAPLUS ABB=ON (L24 OR L25)
 L27 2353 SEA FILE=CAPLUS ABB=ON L26(L) CAT/RL
 L31 6 SEA FILE=CAPLUS ABB=ON L20 AND (L16 OR L27)

L14 152839 SEA FILE=REGISTRY ABB=ON RU/ELS
 L15 101120 SEA FILE=CAPLUS ABB=ON L14
 L16 25439 SEA FILE=CAPLUS ABB=ON L15(L) CAT/RL
 L17 150091 SEA FILE=CAPLUS ABB=ON ALCOHOLS/CT
 L19 18354 SEA FILE=CAPLUS ABB=ON L17(L) PREP/RL
 L22 23387 SEA FILE=CAPLUS ABB=ON "RESOLUTION (SEPARATION)" +OLD/CT
 L24 1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
 L25 1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
 L26 51371 SEA FILE=CAPLUS ABB=ON (L24 OR L25)
 L27 2353 SEA FILE=CAPLUS ABB=ON L26(L) CAT/RL
 L28 995 SEA FILE=CAPLUS ABB=ON DYNAMIC/OBI (L) KINETIC/OBI
 L29 226 SEA FILE=CAPLUS ABB=ON L28(L) L22
 L30 9 SEA FILE=CAPLUS ABB=ON L29 AND (L16 OR L27) AND L19

L14 152839 SEA FILE=REGISTRY ABB=ON RU/ELS
 L15 101120 SEA FILE=CAPLUS ABB=ON L14
 L16 25439 SEA FILE=CAPLUS ABB=ON L15(L) CAT/RL
 L17 150091 SEA FILE=CAPLUS ABB=ON ALCOHOLS/CT
 L19 18354 SEA FILE=CAPLUS ABB=ON L17(L) PREP/RL
 L21 33996 SEA FILE=CAPLUS ABB=ON "ASYMMETRIC SYNTHESIS AND INDUCTION" +OL
 D, NT/CT
 L24 1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
 L25 1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
 L26 51371 SEA FILE=CAPLUS ABB=ON (L24 OR L25)
 L27 2353 SEA FILE=CAPLUS ABB=ON L26(L) CAT/RL
 L35 3653 SEA FILE=CAPLUS ABB=ON CHIRAL/OBI (L) (ALCOHOL/OBI OR ALCS/OBI)
 L38 5627 SEA FILE=CAPLUS ABB=ON ACHIRAL/BI
 L39 3 SEA FILE=CAPLUS ABB=ON L19 AND L35 AND L21 AND (L27 OR L16)
 AND L38

L14 152839 SEA FILE=REGISTRY ABB=ON RU/ELS
 L15 101120 SEA FILE=CAPLUS ABB=ON L14
 L16 25439 SEA FILE=CAPLUS ABB=ON L15(L) CAT/RL
 L17 150091 SEA FILE=CAPLUS ABB=ON ALCOHOLS/CT
 L19 18354 SEA FILE=CAPLUS ABB=ON L17(L) PREP/RL
 L21 33996 SEA FILE=CAPLUS ABB=ON "ASYMMETRIC SYNTHESIS AND INDUCTION" +OL
 D, NT/CT
 L24 1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
 L25 1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
 L26 51371 SEA FILE=CAPLUS ABB=ON (L24 OR L25)
 L27 2353 SEA FILE=CAPLUS ABB=ON L26(L) CAT/RL

L35 3653 SEA FILE=CAPLUS ABB=ON CHIRAL/OBI(L) (ALCOHOL/OBI OR ALCS/OBI)

L41 19466 SEA FILE=CAPLUS ABB=ON ENANTIOSELECT?/OBI

L42 4 SEA FILE=CAPLUS ABB=ON L19(L)L41 AND L35 AND L21 AND (L27 OR L16)

L17 150091 SEA FILE=CAPLUS ABB=ON ALCOHOLS/CT

L19 18354 SEA FILE=CAPLUS ABB=ON L17(L) PREP/RL

L20 136 SEA FILE=CAPLUS ABB=ON L19(L) "S"/OBI

L21 33996 SEA FILE=CAPLUS ABB=ON "ASYMMETRIC SYNTHESIS AND INDUCTION"+OLD D,NT/CT

L22 23387 SEA FILE=CAPLUS ABB=ON "RESOLUTION (SEPARATION)" +OLD/CT

L35 3653 SEA FILE=CAPLUS ABB=ON CHIRAL/OBI(L) (ALCOHOL/OBI OR ALCS/OBI)

L41 19466 SEA FILE=CAPLUS ABB=ON ENANTIOSELECT?/OBI

L43 66509 SEA FILE=CAPLUS ABB=ON KETONES/CT

L44 11738 SEA FILE=CAPLUS ABB=ON RACEMIC/OBI

L45 10 SEA FILE=CAPLUS ABB=ON L43(L)L44 AND L19 AND (L20 OR L21 OR L22 OR L35 OR L41)

=> s 131,130,139,142,145 not 1117

L132 27 (L31 OR L30 OR L39 OR L42 OR L45) NOT L117

=> dup rem 1131,1132

FILE 'CASREACT' ENTERED AT 16:46:51 ON 02 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'CAPLUS' ENTERED AT 16:46:51 ON 02 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
PROCESSING COMPLETED FOR L131
PROCESSING COMPLETED FOR L132

L133 42 DUP REM L131 L132 (2 DUPLICATES REMOVED)
ANSWERS '1-17' FROM FILE CASREACT
ANSWERS '18-42' FROM FILE CAPLUS

=> d ibib abs fh1t

L133 ANSWER 1 OF 42 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 138:271003 CASREACT Full-text

TITLE: Efficient lipase-catalyzed kinetic resolution and dynamic kinetic resolution of β -hydroxy nitriles. Correction of absolute configuration and transformation to chiral β -hydroxy acids and γ -amino alcohols

AUTHOR(S): Pamies, Oscar; Backvall, Jan-E.

CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, 106 91, Swed.

SOURCE: Advanced Synthesis & Catalysis (2002), 344(9), 947-952
CODEN: ASCAF7; ISSN: 1615-4150

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

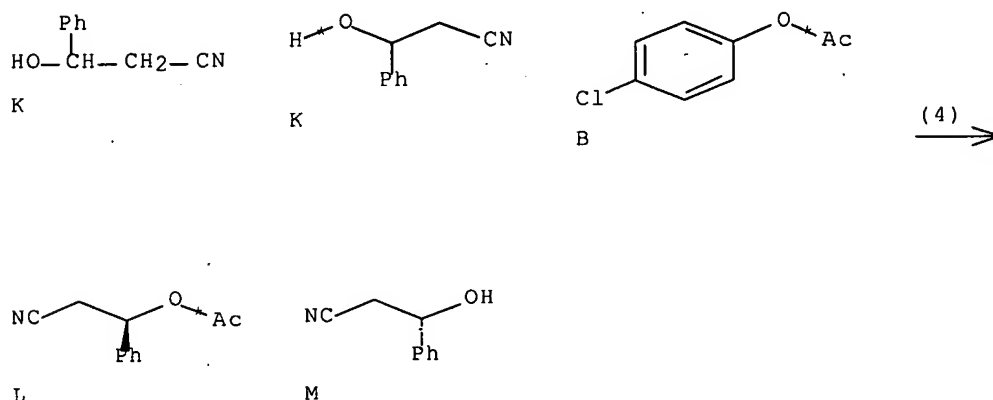
DOCUMENT TYPE: Journal

LANGUAGE: English

not d.

AB Chemoenzymic dynamic kinetic resolution of β -hydroxy nitriles has been carried out using *Candida antarctica* lipase B and a ruthenium catalyst. The use of a hydrogen source to depress ketone formation in the dynamic kinetic resolution yields the acetates in good yield and high enantioselectivity. It is shown that the ruthenium catalyst and the enzyme can be recycled when used in sep. reactions. Enantiomerically pure β -hydroxy acid derivs. and γ -amino alcs. were prepared from the hydroxy nitriles and acetates. The latter compds. were also used to establish the correct absolute configuration of the hydroxy nitriles and acetates.

RX(4) OF 50 2 K + B ==> L + M...



RX(4) RCT K 17190-29-3, B 876-27-7
 PRO L 198561-42-1, M 132203-26-0
 CAT 9001-62-1 Lipase, 104439-77-2 Ruthenium,
 tetracarbonyl- μ -hydro[(1,2,3,4,5- η)-1-hydroxylato-2,3,4,5-
 tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5- η)-1-hydroxy-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
 SOL 108-88-3 PhMe
 CON 24 hours, 60 deg C
 NTE Biotransformation, enzymic, stereoselective
 , kinetic resoln., *Candida antarctica* lipase B (N-435) present as
 catalyst

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs fhit 2-17; d ibib ed abs hitind 18-42; fil hom

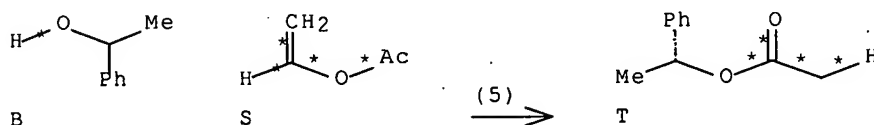
L133 ANSWER 2 OF 42 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 2
 ACCESSION NUMBER: 130:266981 CASREACT Full-text
 TITLE: Ruthenium- and Enzyme-Catalyzed Dynamic Kinetic
 Resolution of Secondary Alcohols
 AUTHOR(S): Persson, B. Anders; Larsson, Anna L. E.; Le Ray,
 Mikael; Baekvall, Jan-E.
 CORPORATE SOURCE: Departments of Organic Chemistry, Uppsala University,
 Uppsala, S-751 21, Swed.
 SOURCE: Journal of the American Chemical Society (1999),

121(8), 1645-1650
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

got 21.

AB Enzymic resolution of secondary alcs. under substrate racemizing conditions was studied using an immobilized lipase from *Candida antarctica* in the presence of a Ru catalyst. A specifically designed acyl donor, 4-chlorophenyl acetate, is compatible with both catalysts and resulted in an efficient dynamic kinetic resolution. Studies of the reaction in different solvents showed that nonpolar solvents gave the best results. With this process, racemic secondary alcs. were transformed to the corresponding enantiomerically pure acetates, making efficient use of all starting material. In most cases, the reaction proceeded with >99% ee and in good yield.

RX(5) OF 37 ...B + S ==> T



RX(5) RCT B 98-85-1, S 108-05-4
 RGT C 98-86-2 Acetophenone
 PRO T 16197-92-5
 CAT 104439-77-2 Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-, 9001-62-1 Lipase
 SOL 75-65-0 t-BuOH
 CON 17 hours, 70 deg C
 NTE **stereoselective**, solid-supported catalyst, **enzymic**, biotransformation, lipase B (Novozyme 435) supported on acrylic resin from *Candida antartica* used, ee >99%, kinetic resolution

REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

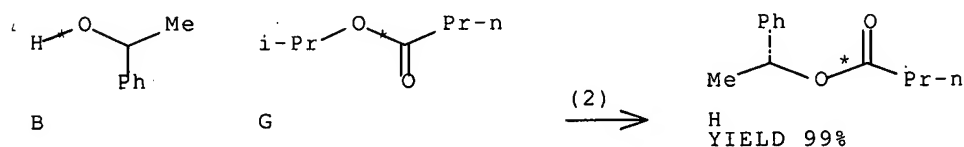
L133 ANSWER 3 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 146:7598 CASREACT Full-text
 TITLE: Efficient dynamic kinetic resolution of secondary alcohols with a novel tetrafluorosuccinato ruthenium complex
 AUTHOR(S): van Nispen, Sjoerd F. G. M.; van Buijtenen, Jeroen; Vekemans, Jef A. J. M.; Meuldijk, Jan; Hulshof, Lumbertus A.
 CORPORATE SOURCE: Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
 SOURCE: Tetrahedron: Asymmetry (2006), 17(15), 2299-2305
 CODEN: TASYE3; ISSN: 0957-4166
 PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Dynamic kinetic resolution (DKR) of a series of secondary alcs. RCH(OH)Me ($\text{R} = \text{n-C}_6\text{H}_{13}, \text{Ph}, 4\text{-MeOC}_6\text{H}_4, 4\text{-F}_3\text{CC}_6\text{H}_4, 2\text{-furyl}$) has been conducted with a novel dinuclear ruthenium complex, bearing tetrafluorosuccinate and rac-BINAP ligands as the racemization catalyst. Novozym 435 has been used as the enzyme, and iso-Pr butyrate as the acyl donor. The catalyst performed optimally at 70 °C. Typically the reaction reached complete conversion within 1 day with 0.1 mol % of racemization catalyst relative to the substrate. The addition of the ketone corresponding to the substrate stabilizes the active Ru complex and, therefore, increases the rate of the reaction.

RX(2) OF 7B + G ==> H



RX(2) RCT B 98-85-1, G 638-11-9
 RGT D 584-08-7 K₂CO₃
 PRO H 89378-61-0
 CAT 878999-28-1 Ruthenium, diaquabis[[1,1'-binaphthalene]-2,2'-diylbis[diphenylphosphine-κP]]dicarbonylbis[μ-tetrafluorobutanedioato(2-)-κO1:κO4]]di-, stereoisomer, 9001-62-1 Lipase
 SOL 108-88-3 PhMe
 CON 23 hours, 70 deg C, 200 mbar
 NTE enzymic, stereoselective, >99% ee

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 4 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 143:365755 CASREACT Full-text
 TITLE: Process for the preparation of enantiomerically enriched esters and alcohols by means of azeotropically dried enzyme compositions
 INVENTOR(S): Verzijl, Gerardus Karel Maria
 PATENT ASSIGNEE(S): DSM Ip Assets B. V., Neth.
 SOURCE: PCT Int. Appl., 32 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095629	A1	20051013	WO 2005-EP3312	20050325
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,				

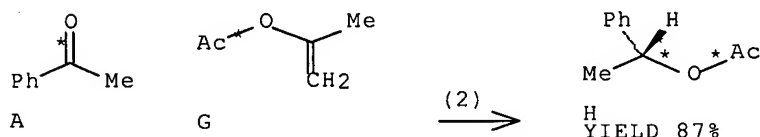
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
 SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
 RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
 MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

EP 2004-75942 20040329

AB Process for the preparation of an enantiomerically enriched ester, which comprises subjecting a mixture of enantiomers of the corresponding secondary alc., in the presence of an acyl donor, to an enantioselective enzymic conversion, wherein the conversion is carried out by using a mixture containing an enantioselective acylating enzyme, which enzyme mixture is prepared by mixing an aqueous solution of the enantioselective acylating enzyme with an organic compound which forms an azeotrope with water and by subsequently azeotropically removing the water.

RX(2) OF 9 A + G ==> H



RX(2) RCT A 98-86-2

STAGE(1)

RGT C 67-63-0 Me₂CHOH

CAT 19196-63-5 Benzeneacetamide, α -amino- α -methyl-,
 584-08-7 K₂CO₃, 52462-29-0 Ruthenium,
 di- μ -chlorodichlorobis[(1,2,3,4,5,6- η)-1-methyl-4-(1-
 methylethyl)benzene]di-

CON 1 hour, 70 deg C

STAGE(2)

RCT G 108-22-5

CAT 9001-62-1 Lipase, 584-08-7 K₂CO₃

SOL 108-88-3 PhMe

CON 24 hours, 70 deg C

PRO H 16197-92-5

NTE biotransformation, enzymic(Novozym 525L used second
 stage), stereoselective(second stage), alternate
 preparations also described, K₂CO₃/enzyme batch can be
 recovered and reused at least four times

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

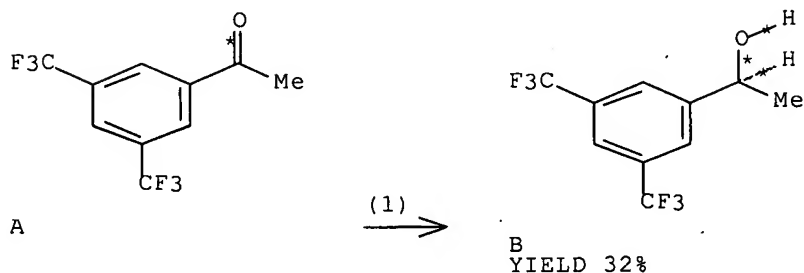
ACCESSION NUMBER: 143:365756 CASREACT Full-text
 TITLE: Chemoenzymic synthesis of chiral secondary alcohols
 INVENTOR(S): Dax, Thomas; Stanek, Michael; Poechlauer, Peter
 PATENT ASSIGNEE(S): DSM Fine Chemicals Austria Nfg GmbH & Co Kg, Austria
 SOURCE: PCT Int. Appl., 21 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095628	A1	20051013	WO 2005-EP1977	20050225
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AT 500556	A1	20060115	AT 2004-471	20040318
EP 1725674	A1	20061129	EP 2005-707624	20050225
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			AT 2004-471	20040318
			WO 2005-EP1977	20050225

OTHER SOURCE(S): MARPAT 143:365756

AB Disclosed is a chemoenzymic method for producing chiral secondary alcs. from ketones. The process consists of a chemical reduction of the ketone to a racemic alc. followed by a lipase catalyzed transesterification of the R-enantiomer. The unreacted S-alc. is then recovered by distillation. The remaining R-ester can then be hydrolyzed and the R-alc may be recycled back into the reaction mixture

RX(1) OF 1 A ==> B



RX(1) RCT A 30071-93-3

STAGE(1)

RGT C 19196-63-5 Benzeneacetamide, α -amino- α -methyl-
 , D 584-08-7 K₂CO₃
 CAT 52462-29-0 Ruthenium, di- μ -
 chlorodichlorobis[(1,2,3,4,5,6- η)-1-methyl-4-(1-
 methylethyl)benzene]di-
 SOL 67-63-0 Me₂CHOH
 CON 1 hour, 85 deg C

STAGE(2)

CAT 9001-62-1 Lipase
 SOL 105-38-4 Propanoic acid, ethenyl ester
 CON 4 hours, 70 deg C, 300 mbar

PRO B 225920-05-8

NTE **stereoselective**, Novozyme435 used in stage 2, second
 stage biotransformation, second stage **enzymic**

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 6 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:381652 CASREACT Full-text

TITLE: How Substrate Solvation Contributes to the
 Enantioselectivity of Subtilisin toward Secondary
 Alcohols

AUTHOR(S): Savile, Christopher K.; Kazlauskas, Romas J.

CORPORATE SOURCE: Department of Chemistry, McGill University, Montreal,
 QC, H3A 2K6, Can.

SOURCE: Journal of the American Chemical Society (2005),
 127(35), 12228-12229

CODEN: JACSAT; ISSN: 0002-7863

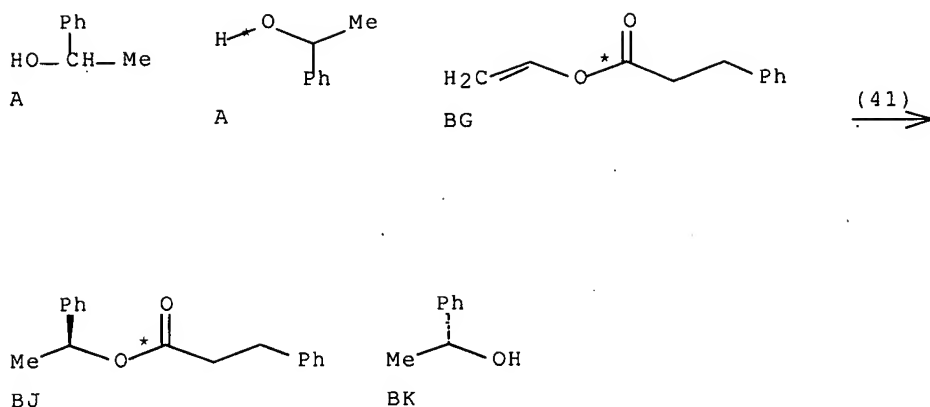
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The current rule to predict the enantiopreference of subtilisin toward
 secondary alcs. is based on the size of the substituents at the stereocenter
 and implies that the active site contains two differently sized pockets for
 these substituents. Several expts. are inconsistent with the current rule.
 First, the X-ray structures of subtilisin show there is only one pocket (the
 S1' pocket) approx. the size of a Ph group to bind secondary alcs. Second,
 the rule often predicts the incorrect enantiomer for reactions in water. To
 resolve these contradictions, we refine the current rule to show that
 subtilisin binds only one substituent of a secondary alc. and leaves the other
 in solvent. To test this refined empirical rule, we show that the
 enantioselectivity of a series of secondary alcs. in water varied linearly
 with the difference in hydrophobicity (log P/P₀) of the substituents. This
 hydrophobicity difference accounts for the solvation of one substituent in
 water.

RX(41) OF 151 ...2 A + BG ==> BJ + BK



RX(41) RCT A 98-85-1, BG 54519-07-2
 PRO BJ 52126-27-9, BK 1517-69-7
 CAT 9014-01-1 Subtilisin
 SOL 123-91-1 Dioxane
 CON >48 hours, 30 deg C
 NTE biotransformation, enzymic(recombinant subtilisin BPN' expressed in protease deficient Bacillus subtilis DB104 used), stereoselective(depends on enzyme and solvent), solid-supported catalyst(KCl)

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 7 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:152899 CASREACT Full-text

TITLE: Combined Ruthenium(II) and Lipase Catalysis for Efficient Dynamic Kinetic Resolution of Secondary Alcohols. Insight into the Racemization Mechanism

AUTHOR(S): Martin-Matute, Belen; Edin, Michaela; Bogar, Krisztian; Kaynak, F. Betuel; Baekvall, Jan-E.

CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, SE-106 91, Swed.

SOURCE: Journal of the American Chemical Society (2005), 127(24), 8817-8825

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

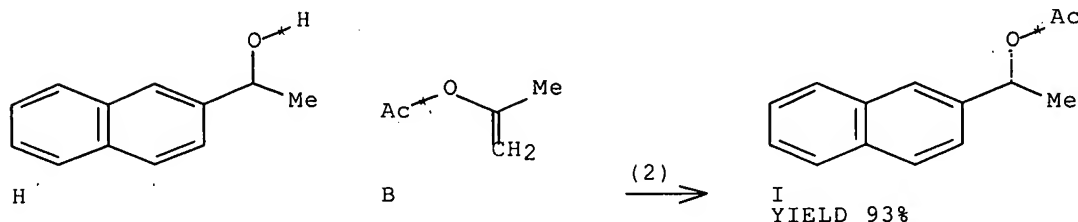
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Pentaphenylcyclopentadienyl ruthenium complexes (3) are excellent catalysts for the racemization of secondary alcs. at ambient temperature. The combination of this process with enzymic resolution of the alcs. results in a highly efficient synthesis of enantiomerically pure acetates at room temperature with short reaction times for most substrates. This new reaction was applied to a wide range of functionalized alcs. including heteroarom. alcs., and for many of the latter, enantiopure acetates were efficiently prepared for the first time via dynamic kinetic resolution (DKR). Different substituted cyclopentadienyl ruthenium complexes were prepared and studied as catalysts for racemization of alcs. Pentaaryl-substituted cyclopentadienyl complexes were found to be highly efficient catalysts for the racemization. Substitution of one of the aryl groups by an alkyl group considerably slows down the racemization process. A study of the racemization of (S)-1-phenylethanol catalyzed by ruthenium hydride $\eta^5\text{-Ph}_5\text{CpRu}(\text{CO})_2\text{H}$ (8) indicates

that the racemization takes place within the coordination sphere of the ruthenium catalyst. This conclusion was supported by the lack of ketone exchange in the racemization of (S)-1-phenylethanol performed in the presence of p-tolyl Me ketone (1 equiv), which gave <1% of 1-(p-tolyl)ethanol. The structures of ruthenium chloride and iodide complexes 3a and 3c and of ruthenium hydride complex 8 were confirmed by X-ray anal.

RX(2) OF 68 H + B ==> I



RX(2)

STAGE(1)

RGT D 865-47-4 t-BuOK, E 497-19-8 Na₂CO₃

CAT 677736-23-1 Ruthenium,

dicarbonylchloro[(1,2,3,4,5-η)-1,2,3,4,5-pentaphenyl-2,4-cyclopentadien-1-yl]-

SOL 108-88-3 PhMe

CON 6 minutes, room temperature

STAGE(2)

RCT H 7228-47-9

CON 4 minutes, room temperature

STAGE(3)

RCT B 108-22-5

CON 3 hours, room temperature

PRO I 84194-78-5

NTE biotransformation, **enzymic**, *Candida antarctica* lipase B
used in stage 1, **stereoselective**

REFERENCE COUNT: 116 THERE ARE 116 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L133 ANSWER 8 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:43627 CASREACT Full-text

TITLE: Dynamic kinetic resolution of secondary alcohols with
a readily available ruthenium-based racemization .
catalyst

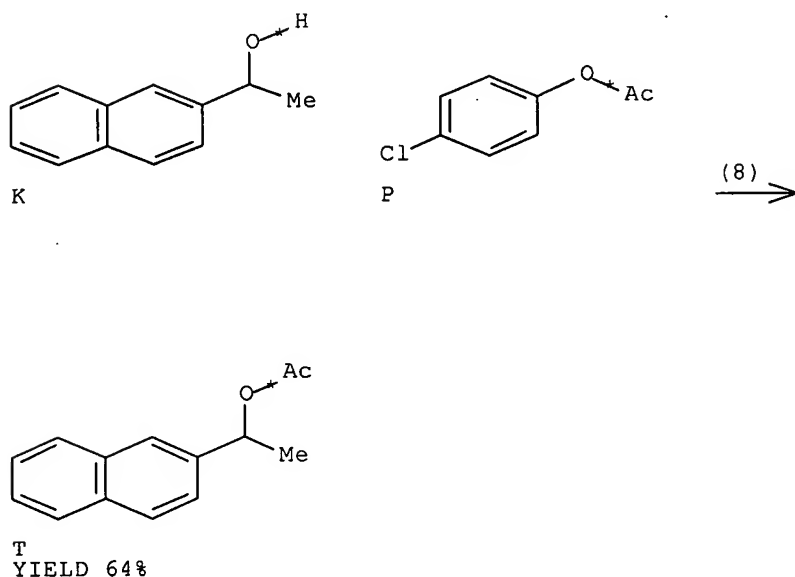
AUTHOR(S): Riermeier, Thomas H.; Gross, Peter; Monsees, Axel;
Hoff, Manfred; Trauthwein, Harald

CORPORATE SOURCE: Degussa AG, Degussa Homogeneous Catalysts,
Hanau-Wolfgang, D-63457, Germany

SOURCE: Tetrahedron Letters (2005), 46(19), 3403-3406
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB An easy to handle and stable racemization catalyst for secondary alcs. is obtained by an in situ mixture of readily available [Ru(cymene)Cl₂]₂ with chelating aliphatic diamines. Optimization of the reaction revealed that N,N,N',N'-tetramethyl-1,3-propanediamine as ligand racemizes aromatic alcs. completely within 5 h. This easy to handle and stable catalytic system is combined with a lipase-catalyzed resolution to provide an efficient dynamic kinetic resolution of secondary alcs.

RX(8) OF 14 ...K + P ==> T



RX(8)

STAGE(1)

CAT 52462-29-0 Ruthenium, di-μ-chlorodichlorobis[(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]di-, 110-95-2 1,3-Propanediamine, N,N,N',N'-tetramethyl-
 SOL 108-88-3 PhMe
 CON 10 minutes, room temperature

STAGE(2)

RCT K 7228-47-9, P 876-27-7
 RGT U 93-08-3 Ethanone, 1-(2-naphthalenyl)-
 CAT 9001-62-1 Lipase
 CON 45 hours, 80 deg C

PRO T 32860-25-6

NTE biotransformation, stereoselective, enzymic

(Candida antarctica B lipase used), dynamic kinetic resolution allows for greater than 50% conversion and yield, lower yield if ketone omitted second stage

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 9 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:76919 CASREACT Full-text

TITLE: Removal of the acyl donor residue allows the use of simple alkyl esters as acyl donors for the dynamic kinetic resolution of secondary alcohols

AUTHOR(S): Verzijl, Gerard K. M.; de Vries, Johannes G.; Broxterman, Quirinus B.

CORPORATE SOURCE: Life Sciences-Advanced Synthesis, Catalysis and Development, DSM Research, Geleen, 6160 MD, Neth.

SOURCE: Tetrahedron: Asymmetry (2005), 16(9), 1603-1610
CODEN: TASYE3; ISSN: 0957-4166

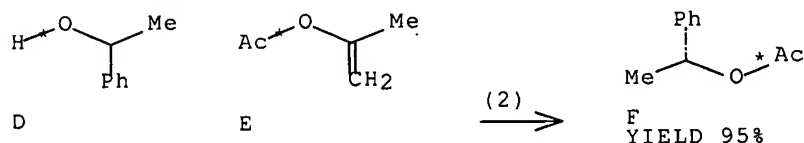
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The dynamic kinetic resolution of secondary alcs. using a lipase and a ruthenium catalyst as developed by Baekvall required some improvements to make it suitable for its use in an industrial process. The use of p-chlorophenyl acetate as acyl donor is not desirable in view of the toxicity of the side product. We herein report that simple alkyl esters can be used as acyl donors if the alc. or ketone residue formed during the enzymic acylation is continuously removed during the reaction. The addition of a ketone speeds up the racemization process and allowed us to reduce the amts. of enzyme and ruthenium catalyst. The scope of this method was explored and a suitable range of acyl donors found. Various benzylic and aliphatic alcs. were reacted using iso-Pr butyrate or Me phenylacetate as acyl donor and in most cases the ester was isolated in >95% yield and 99% ee. Furthermore, it was demonstrated that the alc. byproducts of the enzymic resolution could be used as the hydrogen source in the asym. reductive transesterification of ketones.

RX(2) OF 20 D + E ==> F



RX(2) RCT D 98-85-1, E 108-22-5
PRO F 16197-92-5
CAT 9001-62-1 Lipase, 98-86-2 Acetophenone, 104439-77-2
Ruthenium, tetracarbonyl- μ -hydro[(1,2,3,4,5- η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5- η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
SOL 108-88-3 PhMe
CON 24 hours, 70 deg C, 215 mbar

NTE biotransformation, enzymic, stereoselective,
optimization study(optimized on catalyst ratios, pressure),
alternate preparations also described

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 10 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 144:253689 CASREACT Full-text

TITLE: (S)-selective kinetic resolution and chemoenzymatic
dynamic kinetic resolution of secondary alcohols

AUTHOR(S): Boren, Linnea; Martin-Matute, Belen; Xu, Yongmei;
Cordova, Armando; Baeckvall, Jan-E.

CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory,
Stockholm University, Stockholm, 106 91, Swed.

SOURCE: Chemistry--A European Journal (2005), Volume Date
2006, 12(1), 225-232

CODEN: CEUJED; ISSN: 0947-6539

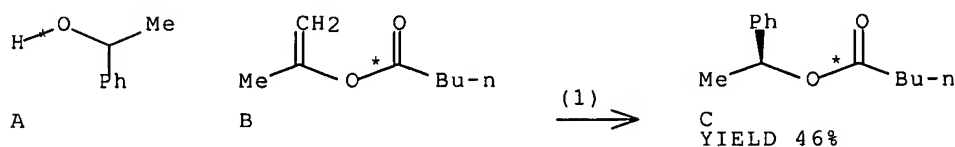
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB (S)-Selective kinetic resolution was achieved through the use of a com.
available protease, which was activated with a combination of two different
surfactants. The kinetic resolution (KR) process was optimized with respect
to activation of the protease and to the acyl donor. The KR proved to be
compatible with a range of functionalized sec-alcs., giving good to high
enantiomeric ratio values (up to >200). The enzymic resolution was combined
with a ruthenium-catalyzed racemization to give an (S)-selective dynamic
kinetic resolution (DKR) of sec-alcs. The DKR process works under very mild
reaction conditions to give the corresponding esters in high yields and with
excellent enantioselectivities.

RX(1) OF 17 A + B ==> C



RX(1) RCT A 98-85-1, B 69638-96-6

RGT D 497-19-8 Na₂CO₃

PRO C 183184-17-0

CAT 9014-01-1 Subtilisin, 29836-26-8 β-D-
Glucopyranoside, octyl, 9004-95-9 Poly(oxy-1,2-ethanediyl),
α-hexadecyl-ω-hydroxy-

SOL 109-99-9 THF

CON 17 hours, room temperature

NTE biotransformation, enzymic, stereoselective, yield depends on
catalyst activator

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 11 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:71330 CASREACT Full-text

TITLE: One-pot synthesis of enantiopure syn-1,3-diacetates from racemic syn/anti mixtures of 1,3-diols by dynamic kinetic asymmetric transformation

AUTHOR(S): Edin, Michaela; Steinreiber, Johannes; Baekvall, Jan-E.

CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, SE-106 91, Swed.

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2004), 101(16), 5761-5766
CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

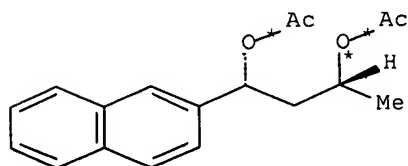
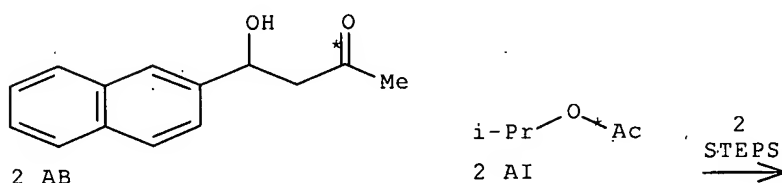
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A one-pot synthesis of enantiomerically pure syn-1,3-diacetates starting from readily accessible racemic diastereomeric mixts. of 1,3-diols has been realized by combining (i) enzymic transesterification, (ii) ruthenium-catalyzed epimerization of a secondary alc. in a diol or diol monoacetate, and (iii) intramol. acyl migration in a syn-1,3-diol monoacetate. The in situ coupling of these three processes results in an efficient enantioselective synthesis of acyclic syn-1,3-diacetates via combined deracemization-deepimerization and constitutes a dynamic kinetic asym. transformation concept. Several differently substituted unsym., acyclic syn-1,3-diacetates were obtained in yields up to 73% with excellent enantioselectivities (>99%) and good diastereomeric ratios (>90% syn).

RX(33) OF 34 COMPOSED OF RX(23), RX(20)

RX(33) 2 AB + 2 AI ==> AM

AM
YIELD 53%

RX(23) RCT AB 229156-79-0

STAGE(1)
 RGT P 16940-66-2 NaBH4
 SOL 67-56-1 MeOH
 CON 1 hour, room temperature

STAGE(2)
 SOL 7732-18-5 Water
 CON room temperature

PRO AL 712342-54-6, AP 712342-65-9
 NTE stereoselective

RX(20) RCT AL 712342-54-6, AI 108-21-4

STAGE(1)
 CAT 104439-77-2 Ruthenium, tetracarbonyl- μ -
 hydro[(1,2,3,4,5- η)-1-hydroxylato-2,3,4,5-tetraphenyl-
 2,4-cyclopentadien-1-yl][(1,2,3,4,5- η)-1-hydroxy-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-, 9001-62-1
 Lipase
 SOL 108-88-3 PhMe
 CON SUBSTAGE(1) 12 hours, 70 deg C
 SUBSTAGE(2) 70 deg C -> room temperature

STAGE(2)
 RGT J 1333-74-0 H2
 CON SUBSTAGE(1) 12 hours, room temperature
 SUBSTAGE(2) 45 hours, 70 deg C

PRO AM 712342-62-6
 NTE biotransformation, enzymic

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 12 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:365670 CASREACT Full-text

TITLE: 5-[4-(1-Hydroxyethyl)phenyl]-10,15,20-
 triphenylporphyrin as a Probe of the Transition-State
 Conformation in Hydrolase-Catalyzed Enantioselective
 Transesterifications

AUTHOR(S): Ema, Tadashi; Jittani, Masahito; Furuie, Kenji; Utaka,
 Masanori; Sakai, Takashi

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of
 Engineering, Okayama University, Tsushima, Okayama,
 700-8530, Japan

SOURCE: Journal of Organic Chemistry (2002), 67(7), 2144-2151
 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

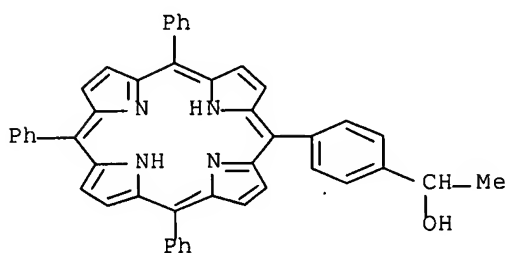
LANGUAGE: English

AB 5-[4-(1-Hydroxyethyl)phenyl]-10,15,20-triphenylporphyrin (1a) and zinc
 porphyrin 1b were designed and synthesized to exptl. examine the validity of
 the transition-state model previously proposed for the lipase-catalyzed
 kinetic resolution of secondary alcs. The lipases from *Pseudomonas cepacia*
 (lipase PS), *Candida antarctica* (CHIRAZYME L-2), *Rhizomucor miehei* (CHIRAZYME
 L-9), and *Pseudomonas aeruginosa* (lipase LIP) exhibited excellent
 enantioselectivity ($E > 100$ at 30°). Subtilisin Carlsberg from *Bacillus*
licheniformis (ChiroCLEC-BL) also showed high enantioselectivity for 1a ($E =$

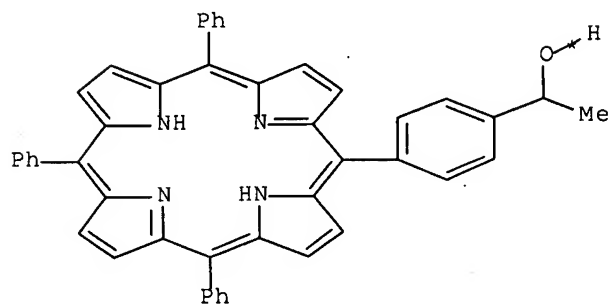
140 at 30°), and the thermodyn. parameters were determined: $\Delta\Delta H_{\text{dbldag.}} = -$

- $6.8 \pm 0.8 \text{ kcal mol}^{-1}$, $\Delta\Delta S_{\text{dbldag.}} = -13 \pm 3 \text{ cal mol}^{-1} \text{ K}^{-1}$. Lipases and subtilisin showed R- and S-preference for 1, resp. The mechanisms underlying the exptl. observations are explained in terms of the transition-state models. The large secondary alc. 1 is a powerful tool for investigating the conformation of the transition state of the enzyme-catalyzed reactions. The fact that 1 was resolved with high enantioselectivity strongly suggests that the gauche conformation, but not the anti conformation, is taken in the transition state, in agreement with the transition-state models involving the stereoelectronic effect.

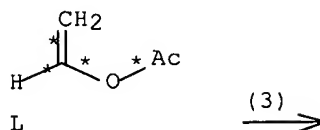
RX(3) OF 10 ... 2 D + L ==> M + N



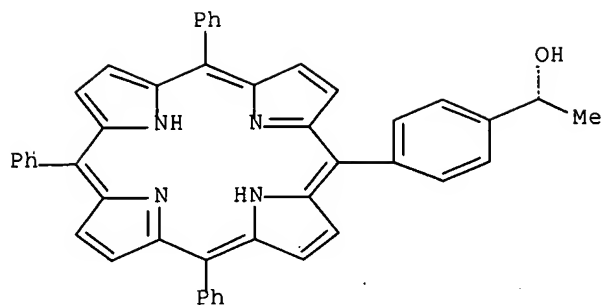
D



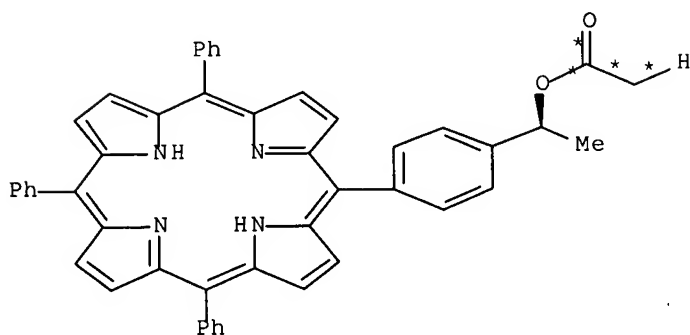
D



(3) →



M



N

RX(3) RCT D 153721-59-6, L 108-05-4
 PRO M 239080-08-1, N 422510-55-2
 CAT 9014-01-1 Subtilisin
 SOL 108-20-3 Isopropyl ether
 NTE enzymic, stereoselective, optimization study, optimized on
 time,temp, resoln. step, sepn. by column chromatog. on silica
 gel

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 13 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 136:4770 CASREACT Full-text

TITLE: Process for the preparation of enantiomerically
 enriched esters and alcohols

INVENTOR(S): Verzijl, Gerardus Karel Maria; De Vries, Johannes
 Gerardus; Broxterman, Quirinus Bernardus

PATENT ASSIGNEE(S): DSM N.V., Neth.

SOURCE: PCT Int. Appl., 43 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND DATE

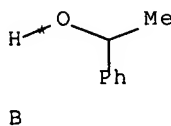
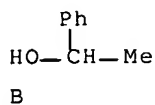
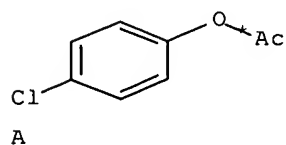
APPLICATION NO. DATE

WO 2001090396	A1	20011129	WO 2001-NL383	20010521
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
NL 1015313	C2	20011127	NL 2000-1015313	20000526
CA 2410529	A1	20011129	CA 2001-2410529	20010521
EP 1283898	A1	20030219	EP 2001-932412	20010521
EP 1283898	B1	20060510		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 200302361	A2	20031028	HU 2003-2361	20010521
JP 2003533993	T	20031118	JP 2001-586591	20010521
AT 325888	T	20060615	AT 2001-932412	20010521
IN 2002CN01933	A	20050211	IN 2002-CN1933	20021125
US 2004077059	A1	20040422	US 2002-296840	20021126
US 6841691	B2	20050111		
PRIORITY APPLN. INFO.:			NL 2000-1015313	20000526
			WO 2001-NL383	20010521

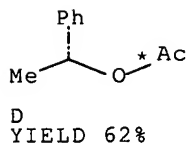
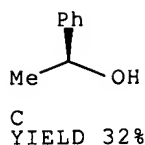
OTHER SOURCE(S): MARPAT 136:4770

AB Method for the preparation of an enantiomerically enriched ester, in which a mixture of the enantiomers of the corresponding secondary alc. is subjected, in the presence of an acyl donor, to an enantioselective conversion in the presence of a racemization catalyst upon which the ester is formed and an acyl donor residue is obtained, and in which the acyl donor residue is irreversibly removed from the phase in which the enantioselective conversion takes place. Preferably the enantioselective conversion is carried out enzymically and a transfer hydrogenation catalyst is used as racemization catalyst. The secondary alc. can be formed in situ from the corresponding ketone, in the presence of a H donor. It is also possible to use a mixture of the secondary alc. and the corresponding ketone as substrate. Preferably the acyl donor is chosen so that the acyl donor residue is converted in situ into another compound and/or the acyl donor residue is removed via distillation under reduced pressure. The enantiomerically enriched esters obtained can subsequently be converted into the corresponding enantiomerically enriched alcs., which are desirable intermediate products in the preparation of liquid crystals, agro chems. or pharmaceuticals.

RX(1) OF 8 A + 2 B ==> C + D



(1) →

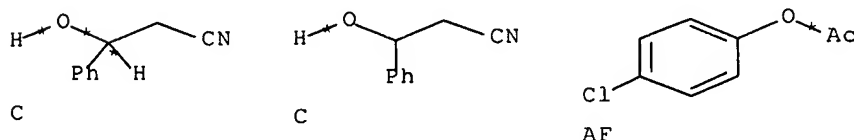


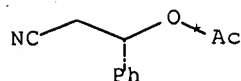
RX(1) RCT A 876-27-7, B 98-85-1
 PRO C 1445-91-6, D 16197-92-5
 CAT 9001-62-1 Lipase, 104439-77-2 Ruthenium,
 tetracarbonyl- μ -hydro[(1,2,3,4,5- η)-1-hydroxylato-2,3,4,5-
 tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5- η)-1-hydroxy-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
 SOL 108-88-3 PhMe
 NTE stereoselective, enzymic, biotransformation,
 alternative prepn.gave lower yields and various selectivity for
 the alc.
 REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 14 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 136:37080 CASREACT Full-text
 TITLE: Efficient lipase-catalyzed kinetic resolution and
 dynamic kinetic resolution of β -hydroxy nitriles.
 A route to useful precursors for γ -amino
 alcohols
 AUTHOR(S): Pamies, Oscar; Backvall, Jan-E.
 CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory,
 Stockholm University, Stockholm, 106 91, Swed.
 SOURCE: Advanced Synthesis & Catalysis (2001), 343(6+7),
 726-731
 CODEN: ASCAF7; ISSN: 1615-4150
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English

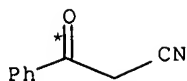
AB An efficient kinetic resolution of racemic β -hydroxy nitriles was performed
 via *Candida antarctica* lipase (N-435)-catalyzed transesterification. A
 variety of racemic alkyl, aryl, and aryloxymethyl substituted β -hydroxy
 nitriles was efficiently transformed to the corresponding enantiomerically
 pure acetates (ee >99% and conversion = 50%) with E values from 40 to >1000.
 The combination of the enzymic kinetic resolution with a ruthenium-catalyzed
 alc. racemization led to a dynamic kinetic resolution (ee's up to 99%, yields
 up to 85%).

RX(13) OF 67 ...2 C + AF ==> AG + AJ





AG
YIELD 74%



AJ
YIELD 23%

RX(13) RCT C 17190-29-3, AF 876-27-7
 PRO AG 21087-76-3, AJ 614-16-4
 CAT 104439-77-2 Ruthenium, tetracarbonyl-μ-
 hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-
 cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-
 tetraphenyl-2,4-cyclopentadien-1-yl]di-, 9001-62-1 Lipase
 SOL 108-88-3 PhMe
 NTE stereoselective, enzymic, candida antarctica
 B (N-435) lipase used, biotransformation, regioselective
 REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 15 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:238582 CASREACT Full-text

TITLE: Effect of crown ethers on structure, stability,
 activity, and enantioselectivity of subtilisin
 carlsberg in organic solvents

AUTHOR(S): Santos, Angelica M.; Vidal, Michael; Pacheco, Yamaris;
 Frontera, Joel; Baez, Carlos; Ornellas, Olivia;
 Barletta, Gabriel; Griebenow, Kai

CORPORATE SOURCE: Department of Chemistry, University of Puerto Rico,
 San Juan, 00931-3346, P. R.

SOURCE: Biotechnology and Bioengineering (2001), 74(4),
 295-308

CODEN: BIBIAU; ISSN: 0006-3592

PUBLISHER: John Wiley & Sons, Inc.

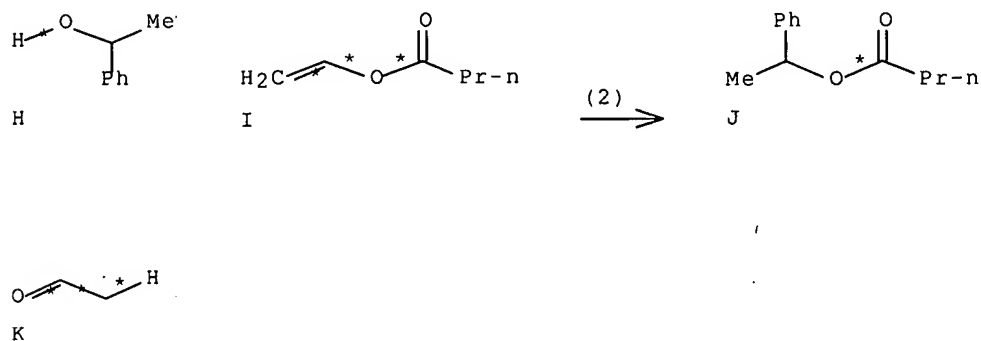
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Co-lyophilization or co-drying of subtilisin Carlsberg with the crown ethers 18-crown-6, 15-crown-5, and 12-crown-4 substantially improved enzyme activity in THF, acetonitrile, and 1,4-dioxane in the transesterification reactions of N-acetyl-L-phenylalanine Et ester and 1-propanol and that of (±)-1-phenylethanol and vinyl butyrate. The acceleration of the initial rate, V_0 , ranged from less than 10-fold to more than 100-fold. All crown ethers activated subtilisin substantially, which excludes a specific macrocyclic effect from being responsible. The secondary structure of subtilisin was studied by Fourier-transform IR (FTIR) spectroscopy. 18-Crown-6 and 15-crown-5 led to a more native-like structure of subtilisin in the organic solvents employed when compared with that of the dehydrated enzyme obtained from buffer alone. However, the high level of activation with 12-crown-4 where this effect was not observed excluded overall structural preservation from being the primary cause of the observed enzyme activation. The conformational mobility of subtilisin was investigated by performing thermal denaturation expts. in 1,4-dioxane. Although only a small effect of temperature on subtilisin structure was observed for the samples prepared with or without 12-crown-4, both 18-crown-6 and 15-crown-5 caused the enzyme to denature at quite

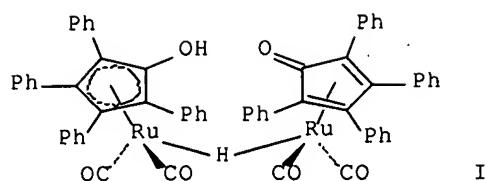
low temps. (38° and 56°, resp.). No relationship between this property and V_o was evident, but increased conformational mobility of the protein decreased its storage stability. The possibility of a "mol. imprinting" effect was also tested by removing 18-crown-6 from the subtilisin-18-crown-6 co-lyophilizate by washing. V_o was only halved as a result of this procedure, an effect insignificant compared with the ca. 80-fold rate enhancement observed prior to washing in THF. This suggests that mol. imprinting is likely the primary cause of subtilisin activation by crown ethers, as recently suggested.

RX(2) OF 2 H + I ==> J + K



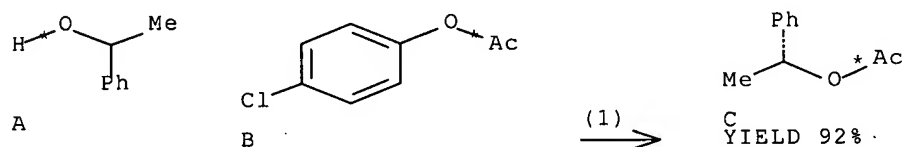
RX(2) RCT H 98-85-1, I 123-20-6
 RGT E 294-93-9 12-Crown-4
 PRO J 3460-44-4, K 75-07-0
 CAT 9014-01-1 Subtilisin
 SOL 109-99-9 THF
 NTE biotransformation, enzymic, optimization study
 REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 16 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 127:135610 CASREACT Full-text
 TITLE: Enzymic resolution of alcohols coupled with
 ruthenium-catalyzed racemization of the substrate
 alcohol
 AUTHOR(S): Larsson, Anna L. E.; Persson, B. Anders; Backvall,
 Jan-E.
 CORPORATE SOURCE: Department Organic Chemistry, Uppsala University,
 Uppsala, S-75121, Swed.
 SOURCE: Angewandte Chemie, International Edition in English
 (1997), 36(11), 1211-1212
 CODEN: ACIEAY; ISSN: 0570-0833
 PUBLISHER: Wiley-VCH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The ruthenium-catalyzed racemization of (+)-(R)- α -methylbenzenemethanol was coupled with an enzyme-catalyzed transesterification to give the resolved alc. derivative. Thus, the combination of catalyst I, 4-chlorophenyl acetate and Novozym 435 in the reaction of (+)-(R)- α -methylbenzenemethanol gave (R)- α -methylbenzenemethanol acetate in high yield and high enantiomeric purity.

RX(1) OF 2 A + B ==> C



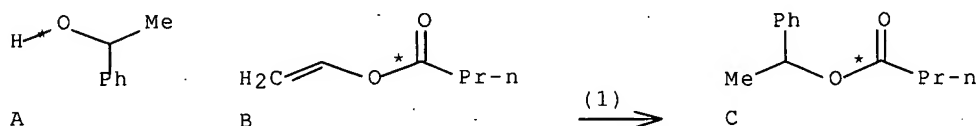
RX(1) RCT A 98-85-1, B 876-27-7
 RGT D 9001-62-1 Lipase
 PRO C 16197-92-5
 CAT 104439-77-2 Ruthenium, tetracarbonyl- μ -hydro[(1,2,3,4,5- η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5- η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
 SOL 75-65-0 t-BuOH
 NTE acetophenone also present, biotransformation, **enzymic**, **stereoselective**, other acetate sources gave lower conversions with equal selectivity
 REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 17 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 114:159632 CASREACT Full-text
 TITLE: How can the solvent affect enzyme enantioselectivity?
 AUTHOR(S): Fitzpatrick, Paul A.; Klibanov, Alexander M.
 CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
 SOURCE: Journal of the American Chemical Society (1991), 113(8), 3166-71
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The enantioselectivity of subtilisin Carlsberg in the transesterification between the chiral alc., sec-phenethyl alc., and vinyl butyrate was found to

be greatly affected by the solvent; e.g., the $(k_{cat}/K_M)S/(k_{cat}/K_M)R$ ratio varied from 3 in anhydrous acetonitrile of 61 in anhydrous dioxane. A mechanistic model was proposed that explained these findings. This model was supported by exptl. data obtained concerning the dependence of subtilisin's enantioselectivity on the structure of the chiral alc., on physicochem. characteristics of the solvent (systematic correlations were found with the dielec. constant and dipole moment), and on such additives as water and the water mimic, formamide. Similar dependencies (although of a smaller magnitude) were observed for the related enzyme, subtilisin BPN'.

RX(1) OF 1 A + B ==> C



RX(1) RCT A 98-85-1, B 123-20-6
 PRO C 3460-44-4
 CAT 9014-01-1 Subtilisin
 NTE Biotransformation: catalyzed by subtilisin

L133 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2006:453821 CAPLUS Full-text
 DOCUMENT NUMBER: 145:62617
 TITLE: Asymmetric transfer hydrogenation of
 α,β -unsaturated, α -tosyloxy and
 α -substituted ketones. [Erratum to document
 cited in CA144:369714]
 AUTHOR(S): Hannedouche, Jerome; Peach, Philip; Cross, David J.;
 Kenny, Jennifer A.; Mann, Inderjit; Houson, Ian;
 Campbell, Lynne; Walsgrove, Tim; Wills, Martin
 CORPORATE SOURCE: Department of Chemistry, University of Warwick,
 Coventry, CV4 7AL, UK
 SOURCE: Tetrahedron (2006), 62(23), 5549
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 16 May 2006
 AB On page 1864, the author line is incorrect; the third author Jerome
 Hannedouche was omitted.
 CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 IT Alcohols, preparation
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (allyl; preparation of α,β -unsatd. ketones and their
 chemoselective, stereoselective, and enantioselective reduction to allylic
 alcs. by transfer hydrogenation in the presence of nonracemic rhodium

- and ruthenium diamine complexes (Erratum))
- IT **Resolution (separation)**
 (kinetic, dynamic; stereoselective and enantioselective preparation of alcs. by transfer hydrogenation and dynamic kinetic resolution of ketones in the presence of nonracemic rhodium and ruthenium diamine complexes (Erratum))
- IT **Alcohols, preparation**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (stereoselective and enantioselective preparation of alcs. and allylic alcs.
 by transfer hydrogenation of ketones, α,β -enones, and α -tosyloxy ketones in the presence of nonracemic rhodium and ruthenium diamine complexes (Erratum))
- IT 12354-85-7, Bis(pentamethylcyclopentadienylrhodium dichloride) 52462-29-0, (p-Cymene)ruthenium(II) chloride dimer 144222-34-4, N-[(1R,2R)-2-Amino-1,2-diphenylethyl]-4-methylbenzenesulfonamide 167316-27-0, (1S,2S)-(+)-N-p-Tosyl-1,2-diphenylethylenediamine 882022-88-0
 RL: CAT (Catalyst use); USES (Uses)
 (stereoselective and enantioselective preparation of alcs. and allylic alcs.
 by transfer hydrogenation of ketones, α,β -enones, and α -tosyloxy ketones in the presence of nonracemic rhodium and ruthenium diamine complexes (Erratum))

L133 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:124021 CAPLUS Full-text

DOCUMENT NUMBER: 144:369675

TITLE: Resolution of Racemic 2-Aminocyclohexanol Derivatives and Their Application as Ligands in Asymmetric Catalysis

AUTHOR(S): Schiffrers, Ingo; Rantanen, Toni; Schmidt, Frank; Bergmans, Werner; Zani, Lorenzo; Bolm, Carsten

CORPORATE SOURCE: Institut fuer Organische Chemie, RWTH Aachen, Aachen, D-52056, Germany

SOURCE: Journal of Organic Chemistry (2006), 71(6), 2320-2331
 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:369675

ED Entered STN: 10 Feb 2006

AB A preparatively easy and efficient protocol for the resolution of racemic 2-aminocyclohexanol derivs. is described, delivering both enantiomers with >99% enantiomeric excess (ee) by sequential use of (R)- and (S)-mandelic acid. A simple aqueous workup procedure permits the isolation of the amino alcs. in anal. pure form and the almost quant. recovery of mandelic acid. Debenzylation of enantiopure trans-2-(benzylamino)-1-cyclohexanol by hydrogenation and subsequent derivatization give access to a broad variety of diversely substituted derivs. Furthermore, the corresponding cis isomers are readily available. Applications of these optically active aminocyclohexanols in catalyzed asym. Ph transfer reactions to benzaldehydes and transfer hydrogenations of aryl ketones lead to products with up to 96% ee.

CC 24-5 (Alicyclic Compounds)

IT **Ketones, reactions**

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkyl aromatic; preparation of enantiopure 2-aminocyclohexanols and analogs)

via resolution of racemic derivs. with mandelic acids and their use as chiral ligands in asym. Ph transfer reaction to benzaldehydes and transfer hydrogenation of aryl ketones)

IT Alcohols, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(benzyl; preparation of enantiopure 2-aminocyclohexanols and analogs via resolution of racemic derivs. with mandelic acids and their use as chiral ligands in asym. Ph transfer reaction to benzaldehydes and transfer hydrogenation of aryl ketones)

IT Alcohols, preparation

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(chiral, amino; preparation of enantiopure 2-aminocyclohexanols and analogs via resolution of racemic derivs. with mandelic acids and their use as chiral ligands in asym. Ph transfer reaction to benzaldehydes and transfer hydrogenation of aryl ketones)

IT Arylation catalysts

Asymmetric synthesis and induction

Resolution (separation)

(preparation of enantiopure 2-aminocyclohexanols and analogs via resolution

of

racemic derivs. with mandelic acids and their use as chiral ligands in asym. Ph transfer reaction to benzaldehydes and transfer hydrogenation of aryl ketones)

REFERENCE COUNT: 217 THERE ARE 217 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:115656 CAPLUS Full-text

DOCUMENT NUMBER: 144:369714

TITLE: Asymmetric transfer hydrogenation of α,β -unsaturated, α -tosyloxy and α -substituted ketones

AUTHOR(S): Peach, Philip; Cross, David J.; Kenny, Jennifer A.; Mann, Inderjit; Houson, Ian; Campbell, Lynne; Walsgrove, Tim; Wills, Martin

CORPORATE SOURCE: Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK

SOURCE: Tetrahedron (2006), 62(8), 1864-1876
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:369714

ED Entered STN: 08 Feb 2006

AB Asym. transfer hydrogenation of cyclic and acyclic α,β -unsatd. ketones catalyzed by ruthenium and rhodium diamine and amino alc. complexes have been investigated. Cyclic α,β -unsatd. ketones appeared to be more suitable substrates for the synthesis of enantiomerically pure allylic alcs. than do acyclic α,β -unsatd. ketones. A proposed mechanism for the formation of 4-phenyl[1,3]-2-dioxolanone from α -tosyloxy- and halo-substituted acetophenone derivs. is discussed. The results of further investigations into the reduction of a range of α -tosyloxyacetophenone derivs. and the dynamic kinetic resolution of α -substituted ketones is presented.

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Alcohols, preparation

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(allyl; preparation of α,β -unsatd. ketones and their chemoselective, stereoselective, and enantioselective reduction to allylic alcs. by transfer hydrogenation in the presence of nonracemic rhodium and ruthenium diamine complexes)

IT Resolution (separation)

(kinetic, dynamic; stereoselective and enantioselective preparation of alcs. by transfer hydrogenation and dynamic kinetic resolution of ketones in the presence of nonracemic rhodium and ruthenium diamine complexes)

IT Alcohols, preparation

Ketones, preparation

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(stereoselective and enantioselective preparation of alcs. and allylic

alcs.

by transfer hydrogenation of ketones, α,β -enones, and α -tosyloxy ketones in the presence of nonracemic rhodium and ruthenium diamine complexes)

IT 12354-85-7, Bis(pentamethylcyclopentadienylrhodium dichloride) 13472-33-8 52462-29-0, (p-Cymene)ruthenium(II) chloride dimer 126456-43-7 144222-34-4, N-[(1R,2R)-2-Amino-1,2-diphenylethyl]-4-methylbenzenesulfonamide 167316-27-0, (1S,2S)-(+)-N-p-Tosyl-1,2-diphenylethylenediamine 882022-88-0

RL: CAT (Catalyst use); USES (Uses)

(stereoselective and enantioselective preparation of alcs. and allylic

alcs.

by transfer hydrogenation of ketones, α,β -enones, and α -tosyloxy ketones in the presence of nonracemic rhodium and ruthenium diamine complexes)

REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:220057 CAPLUS Full-text

DOCUMENT NUMBER: 145:292400

TITLE: Simple and recyclable oxidation, racemization and dynamic kinetic resolution of activated alcohols catalyzed by hydrated ruthenium chloride in aqueous medium

AUTHOR(S): Wolfson, Adi; Yehuda, Chen; Shokin, Olga; Tavor, Dorith

CORPORATE SOURCE: Chemical Engineering Department, Sami Shamoon College of Engineering, Beer Sheva, 84100, Israel

SOURCE: Letters in Organic Chemistry (2006), 3(2), 107-110
CODEN: LOCEC7; ISSN: 1570-1786

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 13 Mar 2006

AB Employing water as medium for aerobic oxidation and dynamic kinetic resolution of activated alcs. with RuCl_3 , NH_2O resulted in simple and recyclable catalytic systems.

CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 7, 67

IT Resolution (separation)

(kinetic, dynamic; recyclable oxidation, racemization and dynamic kinetic resolution, DKR, of activated alcs. catalyzed by hydrated ruthenium chloride in aqueous medium)

IT Alcohols, reactions

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP
(Preparation); RACT (Reactant or reagent)

(recyclable oxidation, racemization and dynamic kinetic resolution, DKR, of
activated alcs. catalyzed by hydrated ruthenium chloride in aqueous medium)

IT 14898-67-0

RL: CAT (Catalyst use); USES (Uses)

(recyclable oxidation, racemization and dynamic kinetic resolution, DKR, of
activated alcs. catalyzed by hydrated ruthenium chloride in aqueous medium)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 22 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1116636 CAPLUS Full-text

DOCUMENT NUMBER: 143:440060

TITLE: Process for preparation of optically pure
water-soluble 1,2-bis[2-(hydroxysulfonyl)phenyl]-1,2-
ethylenediamine derivatives and application as
asymmetric transfer hydrogenation catalysts

INVENTOR(S): Deng, Jingen; Ma, Yaping; Wang, Fei; Zhu, Jin; Cui,
Xin

PATENT ASSIGNEE(S): Chengdu Institute of Organic Chemistry, Chinese
Academy of Sciences, Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 16 pp.
CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1566084	A	20050119	CN 2003-135181	20030612
PRIORITY APPLN. INFO.:			CN 2003-135181	20030612
OTHER SOURCE(S):	CASREACT 143:440060			

ED Entered STN: 18 Oct 2005

AB The invention relates to novel water-soluble diamine and its derivs., their
preparation and application, specifically optically pure 1,2-bis[2-
(hydroxysulfonyl)phenyl]-1,2-ethylenediamine derivs., their preparation and
application in asym. catalysis. By using the ligand and transition metals
(Group VIII) such as ruthenium, rhodium, and iridium as the asym. catalyst in
aqueous phase and water-organic phase transfer hydrogenation, most aryl alkyl
ketones can be hydrogenated with the similar results as in homogeneous phase
catalytic reaction and with ee about 98%, wherein the expected ω -bromo aryl
alkyl alcs. and the epoxy compds. can be obtained from ω -bromo aryl alkyl
ketones by the catalytic reaction in aqueous or water-organic two phase
medium. The catalysts in the invention can be used to get high conversion
rate and unchangeable enantioselectivity even after repeated uses.
Surfactants can accelerate this reaction effectively.

IC ICM C07C309-46

ICS C07C303-06; C07C311-18; C07C303-34; C07C029-143; B01J031-12

CC 25-13 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST enantioselective prepn benzylic alc transfer hydrogenation
chiral amine

IT Ketones, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkyl aromatic; preparation of benzylic alcs. and aryl oxiranes via
enantioselective transfer hydrogenation of aryl alkyl ketones using
water-soluble chiral vicinal diamine as ligand)

IT Alcohols, preparation

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP

(Preparation)

(benzyl; preparation of benzylic alcs. and aryl oxiranes via
enantioselective transfer hydrogenation of aryl alkyl ketones
using water-soluble chiral vicinal diamine as ligand)

IT Epoxides

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP

(Preparation)

(chiral; preparation of benzylic alcs. and aryl oxiranes
via enantioselective transfer hydrogenation of aryl alkyl ketones using
water-soluble chiral vicinal diamine as ligand)

IT **Asymmetric synthesis and induction**

Phase transfer catalysts

(preparation of benzylic alcs. and aryl oxiranes via
enantioselective transfer hydrogenation of aryl alkyl ketones using
water-soluble chiral vicinal diamine as ligand)

IT Bases, reactions

RL: RGT (Reagent); RACT (Reactant or reagent)

(preparation of benzylic alcs. and aryl oxiranes via
enantioselective transfer hydrogenation of aryl alkyl ketones using
water-soluble chiral vicinal diamine as ligand)

IT Hydrogenation

Hydrogenation catalysts

(transfer, stereoselective; preparation of benzylic alcs. and aryl
oxiranes via enantioselective transfer hydrogenation of aryl alkyl
ketones using water-soluble chiral vicinal diamine as ligand)

IT 12354-84-6 37366-09-9 52462-29-0 82091-73-4

RL: CAT (Catalyst use); USES (Uses)

(preparation of benzylic alcs. and aryl oxiranes via
enantioselective transfer hydrogenation of aryl alkyl ketones using
water-soluble chiral vicinal diamine as ligand)

IT 76155-80-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzylic alcs. and aryl oxiranes via
enantioselective transfer hydrogenation of aryl alkyl ketones using
water-soluble chiral vicinal diamine as ligand)

IT 697-64-3P 1517-69-7P 1565-74-8P 20780-54-5P 23357-45-1P

42070-92-8P 52193-85-8P 58287-18-6P 76116-24-0P 86527-10-8P

101219-68-5P 131965-52-1P 162427-79-4P 166239-06-1P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(preparation of benzylic alcs. and aryl oxiranes via
enantioselective transfer hydrogenation of aryl alkyl ketones using
water-soluble chiral vicinal diamine as ligand)

IT 70-11-1 83-33-0 88-15-3 93-08-3 93-55-0 98-59-9, Tosyl chloride
98-86-2, reactions 99-81-0 100-19-6 121-89-1 122-00-9 403-42-9
445-27-2 529-34-0 4254-67-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of benzylic alcs. and aryl oxiranes via
enantioselective transfer hydrogenation of aryl alkyl ketones using
water-soluble chiral vicinal diamine as ligand)

L133 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:580715 CAPLUS Full-text

DOCUMENT NUMBER: 143:248107

TITLE: Preparation of polymer-supported Ru-TsDPEN catalysts
and use for enantioselective synthesis of
(S)-fluoxetine

AUTHOR(S): Li, Yangzhou; Li, Zhiming; Li, Feng; Wang, Quanrui;
Tao, Fanggang

CORPORATE SOURCE: Department of Chemistry, Fudan University, Shanghai, 200433, Peop. Rep. China

SOURCE: Organic & Biomolecular Chemistry (2005), 3(14), 2513-2518
CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:248107

ED Entered STN: 06 Jul 2005

AB Polymer-supported chiral ligands were prepared based on Noyori's (1S,2S)- or (1R,2R)-N-(p-tolylsulfonyl)-1,2-diphenylethylenediamine. The combination with [RuCl₂(p-cymene)]₂ has been shown to exhibit high activities and enantioselectivities for heterogeneous asym. transfer hydrogenation of aromatic ketones with formic acid-triethylamine azeotrope as the hydrogen donor, whereby affording the resp. optically active alcs., the key precursors of chiral fluoxetine. The catalysts can be recovered and reused in three consecutive runs with no significant decline in enantioselectivity. The procedure avoids the plausible contamination of fluoxetine by the toxic transition metal species.

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of polymer-supported Ru-TsDPEN catalysts for enantioselective synthesis of (S)-fluoxetine)

IT 52462-29-0, p-Cymeneruthenium dichloride dimer 863483-33-4D, polymer-supported
RL: CAT (Catalyst use); USES (Uses)
(preparation of polymer-supported Ru-TsDPEN catalysts for enantioselective synthesis of (S)-fluoxetine)

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 24 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:714960 CAPLUS Full-text

DOCUMENT NUMBER: 144:467855

TITLE: Bulky **achiral** triarylphosphines mimic BINAP in Ru(II)-catalyzed asymmetric hydrogenation of ketones

AUTHOR(S): Jing, Qing; Zhang, Xue; Sun, Jie; Ding, Kuiling

CORPORATE SOURCE: State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China

SOURCE: Advanced Synthesis & Catalysis (2005), 347(9), 1193-1197

CODEN: ASCAF7; ISSN: 1615-4150

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:467855

ED Entered STN: 10 Aug 2005

AB Catalysis of the enantioselective hydrogenation of ketones with Ru(II) complexes composed of cheap **achiral** monodentate phosphine ligands in combination with an enantiopure 1,2-diamine, affording a variety of optically active secondary alcs. with high efficiency and enantioselectivity, is reported. The steric impact of **achiral** monophosphine ligands in Ru complexes was found to be a critical factor for the high enantioselectivity of the reaction. This finding throws some light on a long-standing challenge of the

- high cost of chiral bisphosphine ligands, associated with an industrial application of the asym. hydrogenation of ketones.
- CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 22, 67, 75
- ST **chiral secondary alc enantioselective synthesis asym**
hydrogenation ruthenium catalysis; arom prochiral ketone asym
hydrogenation ruthenium catalysis; ruthenium complex **achiral**
triarylphosphine **chiral** diamine crystal mol structure; mol
mechanics ruthenium complex steric hindrance **achiral**
triarylphosphine ligand
- IT **Steric hindrance**
(effect of steric hindrance of **achiral** triarylphosphine
ligands on the enantioselectivity of asym. hydrogenation of ketones
catalyzed by Ru(II) complexes)
- IT **Molecular mechanics**
(mol. structure of a Ru(II) complex with an **achiral**
triarylphosphine ligand and a chiral diamine calculated by mol. mechanics)
- IT **Molecular structure**
(of Ru(II) complexes with **achiral** triarylphosphine ligands
and a chiral diamine)
- IT **Transition metal complexes**
RL: CAT (Catalyst use); PRP (Properties); USES (Uses)
(phosphine; preparation of **chiral** secondary **alcs.** via
asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky
achiral triarylphosphine ligands and a **chiral**
diamine)
- IT **Asymmetric synthesis and induction**
(preparation of **chiral** secondary **alcs.** via asym.
hydrogenation of ketones catalyzed by Ru(II) complexes with bulky
achiral triarylphosphine ligands and a **chiral**
diamine)
- IT **Ketones, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prochiral, aromatic prochiral ketones; preparation of **chiral**
secondary **alcs.** via asym. hydrogenation of ketones catalyzed
by Ru(II) complexes with bulky **achiral** triarylphosphine
ligands and a **chiral** diamine)
- IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(secondary, **chiral**; preparation of **chiral** secondary
alcs. via asym. hydrogenation of ketones catalyzed by Ru(II)
complexes with bulky **achiral** triarylphosphine ligands and a
chiral diamine)
- IT **Hydrogenation**
Hydrogenation catalysts
(stereoselective; preparation of **chiral** secondary **alcs.**
via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with
bulky **achiral** triarylphosphine ligands and a **chiral**
diamine)
- IT **Phosphines**
RL: CAT (Catalyst use); PRP (Properties); USES (Uses)
(transition metal complexes; preparation of **chiral** secondary
alcs. via asym. hydrogenation of ketones catalyzed by Ru(II)
complexes with bulky **achiral** triarylphosphine ligands and a
chiral diamine)
- IT **886446-25-9 886446-34-0**
RL: CAT (Catalyst use); PRP (Properties); USES (Uses)
(crystal structure; preparation of **chiral** secondary **alcs**
. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with
bulky **achiral** triarylphosphine ligands and a **chiral**

- diamine)
 IT 886446-37-3
 RL: CAT (Catalyst use); PRP (Properties); USES (Uses)
 (mol. structure calculated by mol. mechanics; preparation of chiral secondary alcs. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky achiral triarylphosphine ligands and a chiral diamine)
- IT 886446-26-0 886446-36-2
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of chiral secondary alcs. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky achiral triarylphosphine ligands and a chiral diamine)
- IT 88-15-3, 2-Thienyl methyl ketone 93-08-3 93-55-0, Ethyl phenyl ketone 98-80-6, Phenylboric acid 98-86-2, Methyl phenyl ketone, reactions 99-02-5 100-06-1, Methyl 4-methoxyphenyl ketone 122-00-9, Methyl 4-methylphenyl ketone 403-42-9 445-27-2 577-16-2, Methyl 2-methylphenyl ketone 579-74-8, Methyl 2-methoxyphenyl ketone 626-39-1, 1,3,5-Tribromobenzene 941-98-0, 1-Naphthyl methyl ketone 1192-62-7, 2-Furyl methyl ketone 1271-55-2, Ferrocenyl methyl ketone 2142-63-4 2142-68-9 2142-69-0 3506-36-3 17408-14-9 30071-93-3 172975-69-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of chiral secondary alcs. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky achiral triarylphosphine ligands and a chiral diamine)
- IT 103068-20-8P 278600-38-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of chiral secondary alcs. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky achiral triarylphosphine ligands and a chiral diamine)
- IT 7719-12-2, Phosphorus trichloride
 RL: RGT (Reagent); RACT (Reactant or reagent)
 (preparation of chiral secondary alcs. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky achiral triarylphosphine ligands and a chiral diamine)
- IT 613-87-6P, (S)-1-Phenyl propanol 1445-91-6P, (S)-1-Phenyl ethanol 1572-97-0P, (S)-1-(4-MethoxyPhenyl) ethanol 15914-84-8P, (S)-1-(1-Naphthyl) ethanol 27544-18-9P, (S)-1-(2-Naphthyl) ethanol 27948-39-6P, (S)-1-(2-Thienyl) ethanol 33136-66-2P 36296-97-6P 51100-05-1P, (S)-1-(2-MethylPhenyl) ethanol 51154-54-2P, (S)-1-(4-MethylPhenyl) ethanol 101219-73-2P, (S)-1-(4-FluoroPhenyl) ethanol 108100-06-7P, (S)-1-(2-MethoxyPhenyl) ethanol 112653-32-4P, (S)-1-(2-Furyl) ethanol 114446-55-8P, (S)-1-(2-BromoPhenyl) ethanol 127852-27-1P, (S)-1-(2-TrifluoromethylPhenyl) ethanol 131864-71-6P, (S)-1-(2-ChloroPhenyl) ethanol 134615-22-8P, (S)-1-(3-BromoPhenyl) ethanol 135145-34-5P, (S)-1-(3-ChloroPhenyl) ethanol 171032-87-4P, (S)-1-(2-FluoroPhenyl) ethanol 225920-05-8P, (S)-1-[3,5-Bis(Trifluoromethyl)Phenyl] ethanol 561068-06-2P 886232-53-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of chiral secondary alcs. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky achiral triarylphosphine ligands and a chiral diamine)
- IT 67-63-0, Iso-propanol, uses
 RL: NUU (Other use, unclassified); USES (Uses)

(solvent; preparation of chiral secondary alcs. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky achiral triarylphosphine ligands and a chiral diamine)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 25 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:6908 CAPLUS Full-text

DOCUMENT NUMBER: 145:418744

TITLE: The synthesis of ortho-keto-substituted N,N-dimethyl-(S)-1-phenethylamines

AUTHOR(S): Shishkina, I. N.; Kuznetsova, A. A.; Demyanovich, V. M.; Potekhin, K. A.

CORPORATE SOURCE: Kafedra Org. Khim., Mosk. Gos. Univ., Moscow, Russia

SOURCE: Vestnik Moskovskogo Universiteta, Seriya 2: Khimiya (2005), 46(5), 345-348

CODEN: VMUKA5; ISSN: 0579-9384

PUBLISHER: Izdatel'stvo Moskovskogo Universiteta

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 145:418744

ED Entered STN: 05 Jan 2006

AB A series of (S)-o-acyl- α ,N,N-trimethylbenzylamines (acyl = benzoyl, pivaloyl, p-toluoyl, etc.) were synthesized by condensation of ortho-lithiated (S)- α ,N,N-trimethylbenzylamine with the corresponding acyl chlorides. Three methods for the reduction of the resulting amino ketones, i.e. with LiAlH₄, with LiAlH(OBu-t)₃ or with D-tartaric acid-modified NaBH₄, were investigated; the latter method is shown to be superior for the diastereomeric purity of the products. The amino alcs. prepared were used as chiral catalysts in enantioselective addition of Et₂Zn to benzaldehyde providing (R)-1-phenylethanol in 35-79% ee's.

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST ketone amino prepn redn; amino alc prepn chiral catalyst asym addn diethylzinc benzaldehyde; phenylethylamine ortho lithiation acylation acyl chloride

IT Ketones, preparation

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(amino; preparation of non-racemic ortho-acyl- α ,N,N-trimethylbenzylamines by ortho-lithiation of α ,N,N-trimethylbenzylamine followed by trapping with acyl chlorides)

IT Alcohols, preparation

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(amino; preparation of ortho-(hydroxyalkyl)- α ,N,N-trimethylbenzylamines by reduction of non-racemic o-acyl- α ,N,N-trimethylbenzylamines and their use as catalysts for asym. addition of diethylzinc to benzaldehyde)

IT Asymmetric synthesis and induction

(preparation of ortho-(hydroxyalkyl)- α ,N,N-trimethylbenzylamines by reduction of non-racemic o-acyl- α ,N,N-trimethylbenzylamines and their use as catalysts for asym. addition of diethylzinc to benzaldehyde)

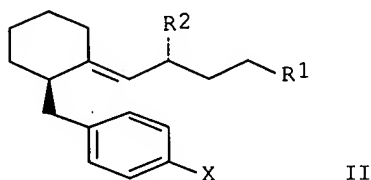
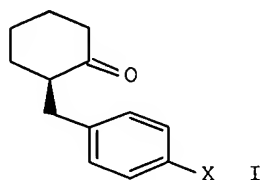
L133 ANSWER 26 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:127619 CAPLUS Full-text

DOCUMENT NUMBER: 142:373286

TITLE: A Chiral Cyclohexanone Linked to Polystyrene for Solid-Phase Synthesis of Chiral α -Carbonyls

AUTHOR(S): Spino, Claude; Gund, Vitthal Genbhau; Nadeau, Christian
 CORPORATE SOURCE: Departement of Chimie, Universite of Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.
 SOURCE: Journal of Combinatorial Chemistry (2005), 7(2), 345-352
 CODEN: JCCHFF; ISSN: 1520-4766
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:373286
 ED Entered STN: 15 Feb 2005
 GI



- AB Two chiral cyclohexanones were linked to polystyrene resin. The polymer-bound auxiliaries were subjected to a sequence of four reactions, the last of which cleaves the desired α -chiral carbonyl compound off the resin, concurrently regenerating the resin-bound auxiliary in its original form. Thus, addition of vinylolithiums, derived from alkenyl iodides $R_1CH_2CH_2CH:CHI$ ($R_1 = n\text{-Pr, Ph, Me}_3\text{CSiMe}_2\text{O}$), to the resin-bound cyclohexanone I ($X = \text{resin}$) followed by chloroformylation / cuprate addition gave the resin-bound alkylidenecyclohexanes II ($R_2 = \text{Me, Me}_3\text{C, Ph, 1-naphthyl, etc.}$), which were cleaved by ozonation to give, after reduction of oxidation if required, a set of non-racemic alcs., aldehydes and carboxylic acids $ZCHR_2CH_2CH_2R_1$ ($Z = \text{HOCH}_2, \text{CHO, HO}_2\text{C}$). The resin can then be reused.
- CC 21-2 (General Organic Chemistry)
- ST cyclohexanone polystyrene linked chiral auxiliary carbonyl compd
 asym synthesis; aldehyde branched solid phase asym synthesis; alc
 branched solid phase asym synthesis; carboxylic acid branched solid phase
 asym synthesis
- IT Carboxylic acids, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (aliphatic; asym. solution and solid-phase synthesis of branched alcs
 ., aldehydes and carboxylic acids using non-racemic cyclohexanones as
 chiral auxiliaries)
- IT Asymmetric synthesis and induction
 Chiral auxiliary
 Solid phase synthesis
 (asym. solution and solid-phase synthesis of branched alcs.,
 aldehydes and carboxylic acids using non-racemic cyclohexanones as
 chiral auxiliaries)
- IT Aldehydes, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (asym. solution and solid-phase synthesis of branched alcs.,
 aldehydes and carboxylic acids using non-racemic cyclohexanones as
 chiral auxiliaries)
- IT Alcohols, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)

- (chiral; asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT Ketones, preparation
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (cycloalkanones; asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT Alkylation
 (stereoselective; asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT 1119-51-3, 5-Bromo-1-pentene 2398-37-0, 3-Methoxyphenyl bromide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Grignard preparation; asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT 98-80-6, Phenylboronic acid 108-86-1, Bromobenzene, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (Suzuki coupling; asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT 77857-39-7P
 RL: BYP (Byproduct); PREP (Preparation)
 (asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT 89-82-7, (+)-Pulegone 94-66-6, 2-Allylcyclohexanone 589-15-1, 4-Bromobenzyl bromide 24347-58-8 25015-63-8, Pinacolborane 77857-35-3 106380-46-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT 53045-12-8P 60595-37-1P, (E)-1-Iodo-1-heptene 67074-37-7P 77857-39-7DP, polystyrene-supported 108330-00-3P 184370-59-0P
 322640-09-5P 849435-82-1P 849435-83-2P 849435-84-3P 849435-85-4P
 849435-88-7P 849435-89-8P 849435-90-1P 849435-91-2P 849435-93-4P
 849435-94-5P 849435-95-6P 849435-96-7P 849435-97-8P 849435-98-9P
 849435-99-0P 849436-01-7P 849436-03-9P 849436-04-0P 849436-10-8P
 849436-21-1P 849436-25-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT 122-97-4P, 3-Phenyl-1-propanol 1949-41-3P 3023-61-8P 17296-92-3P 17297-03-9P 21490-50-6P 40654-82-8P 80651-37-2P 101711-91-5P
 128441-03-2P 194922-80-0P 356784-34-4P 494844-20-1P 849435-86-5P
 849435-87-6P 849435-92-3P 849436-00-6P 849436-02-8P 849436-05-1P
 849436-06-2P 849436-07-3P 849436-08-4P 849436-09-5P 849436-11-9P
 849436-12-0P 849436-13-1P 849436-14-2P 849436-15-3P 849436-16-4P
 849436-17-5P 849436-18-6P 849436-19-7P 849436-20-0P 849436-22-2P
 849436-23-3P 849436-24-4P 849487-55-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (asym. solution and solid-phase synthesis of branched alcs., aldehydes and carboxylic acids using non-racemic cyclohexanones as chiral auxiliaries)
- IT 628-71-7, 1-Heptyne 1823-14-9, 5-Phenyl-1-pentyne 78592-82-2

218434-90-3

RL: RCT (Reactant); RACT (Reactant or reagent) .

(hydroiodination; asym. solution and solid-phase synthesis of branched
alcs., aldehydes and carboxylic acids using non-racemic
cyclohexanones as chiral auxiliaries)

REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 27 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:831386 CAPLUS Full-text

DOCUMENT NUMBER: 142:38128

TITLE: Conversion of chiral unsaturated cyanohydrins into
chiral carba- and heterocycles via ring-closing
metathesis

AUTHOR(S): van den Nieuwendijk, Adrianus M. C. H.; Ghisaidoobe,
Amar B. T.; Overkleeft, Herman S.; Brussee, Johannes;
van der Gen, Arne

CORPORATE SOURCE: Leiden Institute of Chemistry, Gorlaeus Laboratories,
Leiden University, Leiden, 2300 RA, Neth.

SOURCE: Tetrahedron (2004), 60(46), 10385-10396

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

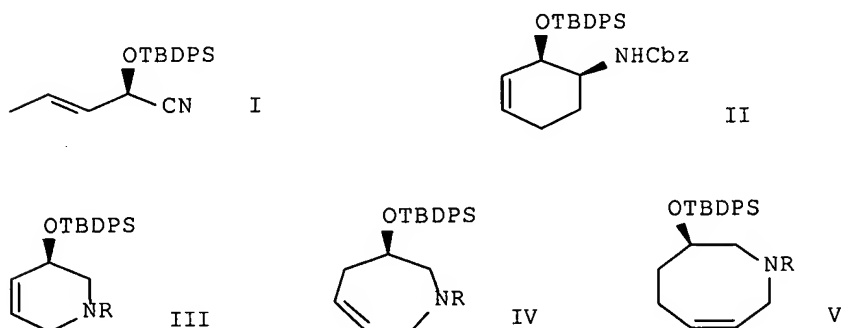
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:38128

ED Entered STN: 12 Oct 2004

GI



AB Aliphatic unsatd. cyanohydrins, e.g., I, served as starting materials in the synthesis of a set of new chiral unsatd. cyclic 1,2-ethanolamines. Combining a Grignard addition-NaBH₄ reduction sequence with a ring-closing metathesis afforded unsatd. cyclic 1,2-ethanolamines, e.g., II, in good yields and high ee (96-99%). The conversion of cyanohydrins via a DIBAL reduction-transimination-NaBH₄ reduction sequence, using allylamine, followed by ring-closing metathesis yielded tetrahydropyridines III (R = Cbz, Boc, Bn), tetrahydroazepinols IV and tetrahydroazocinols V (R = Cbz, Boc) in high yields and excellent ee (97-99%).

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))

IT Alcohols, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(amino, cyclic chiral; stereoselective preparation of chiral unsatd. cyclic
ethanolamines via Grignard addition to chiral silylcyanohydrins followed
by in situ reduction and N-protection with subsequent ring-closing

metathesis catalyzed by Grubb's catalyst)

IT 172222-30-9
 RL: CAT (Catalyst use); USES (Uses)
 (stereoselective preparation of chiral unsatd. cyclic ethanolamines via Grignard addition to chiral silylcyanohydrins followed by in situ reduction and N-protection with subsequent ring-closing metathesis catalyzed by Grubb's catalyst)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 28 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:61086 CAPLUS Full-text

DOCUMENT NUMBER: 140:235450

TITLE: Highly Enantioselective Asymmetric Hydrogenation of α -Phthalimide Ketone: An Efficient Entry to Enantiomerically Pure Amino Alcohols

AUTHOR(S): Lei, Aiwen; Wu, Shulin; He, Minsheng; Zhang, Xumu

CORPORATE SOURCE: Department of Chemistry, Pennsylvania State University, University Park, PA, 16802, USA

SOURCE: Journal of the American Chemical Society (2004), 126(6), 1626-1627

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

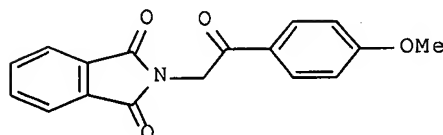
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:235450

ED Entered STN: 26 Jan 2004

GI



I

AB A new type of α -phthalimide ketones, e.g. I, was hydrogenated in excellent enantioselectivity by using a Ru-(C3-TunePhos) complex as the catalyst. Up to 10 000 turnovers have been achieved in more than 99% ee in the hydrogenation reaction. A dynamic kinetic resolution study for the synthesis of threonine was performed, and high anti selectivity (>97:3) was observed for the first time. An efficient method to synthesize enantiomerically pure amino alcs. has been developed.

CC 25-8 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Alcohols, preparation
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (amino; preparation of amino alcs. via Ru-catalyzed enantioselective asym. hydrogenation of α -phthalimide ketone)

IT Resolution (separation)
 (kinetic, dynamic; formation of optically pure allo-threonine derivs. via Ru-catalyzed enantioselective asym. hydrogenation of α -phthalimide ketone)

IT 503114-19-0 668422-82-0
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of amino alcs. via Ru-catalyzed enantioselective asym. hydrogenation of α -phthalimide ketone)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:846735 CAPLUS Full-text
 DOCUMENT NUMBER: 142:354931
 TITLE: A convenient synthesis of optically active unhindered aliphatic alcohols with high optical purity from non-racemic β -hydroxy sulfides
 AUTHOR(S): Cho, Byung Tae; Kim, Dong Jun
 CORPORATE SOURCE: Department of Chemistry, Hallym University, Chunchon, 200-702, S. Korea
 SOURCE: Bulletin of the Korean Chemical Society (2004), 25(9), 1385-1391
 CODEN: BKCSDE; ISSN: 0253-2964
 PUBLISHER: Korean Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 142:354931
 ED Entered STN: 15 Oct 2004
 AB A general route for the synthesis of optically active unhindered aliphatic alcs., where the steric demands between two alkyl groups adjacent to the carbinol are similar, with high enantiomeric purity has been developed by sulfoxidn. of chiral β -hydroxy sulfides, followed by alkylation and desulfurization.
 CC 23-7 (Aliphatic Compounds)
 IT **Alcohols, preparation**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (aliphatic; synthesis of optically active unhindered aliphatic alcs. with high optical purity from non-racemic β -hydroxy sulfides)
 IT **Asymmetric synthesis and induction**
 Reduction
 (synthesis of optically active unhindered aliphatic alcs. with high optical purity from non-racemic β -hydroxy sulfides)
 IT **Ketones, reactions**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis of optically active unhindered aliphatic alcs. with high optical purity from non-racemic β -hydroxy sulfides)
 REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:70318 CAPLUS Full-text
 DOCUMENT NUMBER: 140:253304
 TITLE: Palladium-catalyzed oxidative kinetic resolution with ambient air as the stoichiometric oxidation gas
 AUTHOR(S): Bagdanoff, Jeffrey T.; Stoltz, Brian M.
 CORPORATE SOURCE: The Arnold and Mabel Beckman Laboratories of Chemical Synthesis, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, 91125, USA
 SOURCE: Angewandte Chemie, International Edition (2004), 43(3), 353-357
 CODEN: ACIEF5; ISSN: 1433-7851
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:253304
 ED Entered STN: 29 Jan 2004

AB Air was enough to mediate the enantioselective oxidation of secondary alcs. at room temperature with palladium(II) and sparteine in nonflammable solvents. Examination of the role of solvents capable of hydrogen bonding and their ability to solvate halide anions, led to a set of conditions for the enantioselective oxidative kinetic resolution of secondary alcs.

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 75, 78

ST alc oxidative kinetic resoln; ketone prepn; **chiral**
alc prepn; palladium oxidative kinetic resoln catalyst

IT **Ketones; preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(aromatic; preparation of ketones via palladium-catalyzed oxidative kinetic resolution of **racemic** alcs.)

IT **Resolution (separation)**
(kinetic, oxidative; stereoselective preparation of alcs. via palladium-catalyzed oxidative kinetic resolution of **racemic** alcs.)

IT **Alcohols, preparation**
RL: PUR (Purification or recovery); SPN (Synthetic preparation); **PREP** (Preparation)
(secondary, **chiral**; stereoselective preparation of **alcs.** via palladium-catalyzed oxidative kinetic resolution of **racemic** alcs.)

IT **Asymmetric synthesis and induction**
(stereoselective preparation of alcs. via palladium-catalyzed oxidative kinetic resolution of **racemic** alcs.)

IT 1517-69-7, (+)-1-Phenylethanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of acetophenone via palladium-catalyzed oxidation of **chiral** phenylethanol in the evaluation of solvents for the oxidative kinetic resolution of **racemic** alcs.)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:995754 CAPLUS Full-text

DOCUMENT NUMBER: 140:163517

TITLE: Efficient Heterogeneous Asymmetric Transfer Hydrogenation of Ketones Using Highly Recyclable and Accessible Silica-Immobilized Ru-TsDPEN Catalysts

AUTHOR(S): Liu, Pei Nian; Gu, Pei Ming; Wang, Fei; Tu, Yong Qiang

CORPORATE SOURCE: Department of Chemistry and State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China

SOURCE: Organic Letters (2004), 6(2), 169-172
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

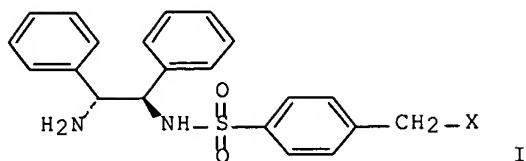
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:163517

ED Entered STN: 23 Dec 2003

GI



- AB Chiral Ru-TsDPEN [N-(p-toluenesulfonyl)-1,2-diphenylethylenediamine] (I, X = H)-derived catalysts were first successfully immobilized onto amorphous silica gel and mesoporous silicas of MCM-41 and SBA-15 by an easily accessible approach. The silica-immobilized catalyst (I; X = CH₂-Silica) demonstrated remarkably high catalytic activities and excellent enantioselectivities (up to >99% ee) for the heterogeneous asym. transfer hydrogenation of various ketones. Particularly, the catalyst could be readily recovered and reused in multiple consecutive catalytic runs (up to 10 uses) with the completely maintained enantioselectivity.
- CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
- ST arom ketone asym transfer hydrogenation **chiral** ruthenium;
alc secondary arom enantioselective prepn; asym transfer
hydrogenation catalyst ruthenium **chiral**
toluenesulfonyldiphenylethylenediamine silica immobilization
- IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aromatic; enantioselective preparation of aromatic alcs. via asym.
transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized
chiral Ru-TsDPEN complexes)
- IT **Asymmetric synthesis and induction**
(enantioselective preparation of aromatic alcs. via asym. transfer
hydrogenation of aromatic ketones catalyzed by silica-immobilized
chiral Ru-TsDPEN complexes)
- IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(secondary, **chiral**, aromatic; enantioselective preparation
of aromatic alcs. via asym. transfer hydrogenation of aromatic
ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN
complexes)
- IT Hydrogenation
Hydrogenation catalysts
(transfer, stereoselective; enantioselective preparation of aromatic
alcs. via asym. transfer hydrogenation of aromatic ketones
catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)
- IT 52462-29-0
RL: CAT (Catalyst use); USES (Uses)
(enantioselective preparation of aromatic alcs. via asym. transfer
hydrogenation of aromatic ketones catalyzed by silica-immobilized
chiral Ru-TsDPEN complexes)
- IT 144222-34-4DP, silica-bound
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)
(enantioselective preparation of aromatic alcs. via asym. transfer
hydrogenation of aromatic ketones catalyzed by silica-immobilized
chiral Ru-TsDPEN complexes)
- IT 83-33-0, 1-Indanone 93-08-3 98-86-2, Acetophenone, reactions
445-27-2, 2'-Fluoroacetophenone 455-36-7 529-34-0, 1-Tetralone
586-37-8 614-16-4, α -Cyanoacetophenone 1192-62-7,
2-Furylmethylketone 2142-68-9, 2'-Chloroacetophenone 2142-69-0,

2'-Bromoacetophenone

RL: RCT (Reactant); RACT (Reactant or reagent)

(enantioselective preparation of aromatic alcs. via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized chiral Ru-TsDPEN complexes)

IT 697-64-3P 1517-69-7P 23357-45-1P 27948-61-4P 52193-85-8P
 73627-97-1P 76116-20-6P 120466-66-2P 120523-12-8P 126534-33-6P
 162427-79-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(enantioselective preparation of aromatic alcs. via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized chiral Ru-TsDPEN complexes)

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 32 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:277075 CAPLUS Full-text

DOCUMENT NUMBER: 138:304045

TITLE: Preparation of ruthenium diphosphine diamine hydride complexes and preparation of alcohols under base-free conditions and optical resolution of racemic carbonyl compounds using the prepared ruthenium hydride complexes

INVENTOR(S): Okuma, Takeshi; Koizumi, Masatoshi; Muniz, Kilian; Noyori, Ryoji

PATENT ASSIGNEE(S): Nagoya Sangyo Kagaku Kenkyusho, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

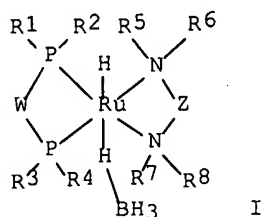
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003104993	A	20030409	JP 2001-301852	20010928
US 6720439	B1	20040413	US 2002-291611	20021112
PRIORITY APPLN. INFO.:			JP 2001-301852	A 20010928

OTHER SOURCE(S): MARPAT 138:304045
 ED Entered STN: 10 Apr 2003
 GI



AB The title complexes I [W = (un)substituted binaphthyl connected to P at 2- or 2'-position; R1-R4 = (un)substituted hydrocarbyl; R1R2 and/or R3R4 may form ring; R5-R8 = H, (un)substituted hydrocarbyl; Z = (un)substituted hydrocarbyl] are prepared Alcs. are prepared by reduction of carbonyl compds. with H or with H donors in the presence of Ru hydride complexes in the absence of strong

bases. Racemic carbonyl compds. are optically resolved by selective reduction of one enantiomer in the presence of Ru hydride complexes. Thus, acetophenone was hydrogenated with H in the presence of {trans-RuH(η^1 -BH₄)[(S)-xylbinap][(S,S)-dpen]} [(S)-xylbinap = (S)-2,2'-bis(di-3,5-xylylphosphino)-1,1'-binaphthyl, (S,S)-dpen = (S,S)-1,2-diphenylethylenediamine] in i-PrOH at 25° for 12 h to give 95% (R)-1-phenylethanol with 99% e.e.

- IC ICM C07F009-50
ICS B01J031-24; C07B041-02; C07C029-145; C07C033-03; C07C033-22; C07C035-08; C07C041-26; C07C041-44; C07C043-196; C07C045-85; C07C049-403; C07C067-31; C07C069-732; C07C069-84; C07C211-27; C07C213-00; C07C215-30; C07D301-00; C07D301-32
- CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 29, 67
- IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amino; optical resolution of racemic carbonyl compds. by reduction using Ru diphosphine diamine hydride complexes)
- IT Alcohols, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(chiral; preparation of alcs. by hydrogenation of carbonyl compds. using Ru diphosphine diamine hydride complex catalysts)
- IT Ketones, preparation
RL: PUR (Purification or recovery); PREP (Preparation)
(optical resolution of racemic carbonyl compds. by reduction using Ru diphosphine diamine hydride complexes)

L133 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:509919 CAPLUS Full-text
DOCUMENT NUMBER: 139:77882
TITLE: Novel ruthenium complexes and process for preparing alcoholic compounds using these
INVENTOR(S): Kuniyiko, Tsutsumi; Kuniyiko, Murata; Takeshi, Ota; Takao, Ikariya
PATENT ASSIGNEE(S): Kanto Kagaku Kabushiki Kaisha, Japan
SOURCE: Eur. Pat. Appl., 28 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1323724	A2	20030702	EP 2002-28791	20021223
EP 1323724	A3	20030924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2003252884	A	20030910	JP 2002-248058	20020828
JP 3566955	B2	20040915		
CA 2414265	A1	20030628	CA 2002-2414265	20021216
US 2003166978	A1	20030904	US 2002-330501	20021227
US 6790973	B2	20040914		

PRIORITY APPLN. INFO.: JP 2001-401170 A 20011228
JP 2002-248058 A 20020828

OTHER SOURCE(S): MARPAT 139:77882

ED Entered STN: 04 Jul 2003

AB Claimed are optically active Ru diphosphine complexes which have asymmetry on carbon, Ru(X)(Y)(R₅R₆PCHR₁CR₃R₄CHR₂PR₇R₈) (1, wherein X and Y represent a H

atom or an anion group, R1 and R2 represent a chain or cyclic hydrocarbon C1-20 group which can be substituted, R3 and R4 represent a H atom or a hydrocarbon C1-3 group, and R5, R6, R7 and R8 represent a hydrocarbon C1-30 group which can be substituted, with the proviso that when X and Y are Br, R1 and R2 are a Me group, and when R3 and R4 are a H atom, at least one of R5, R6, R7 and R8 is not a Ph group.), and optically active Ru diphosphine diamine complexes Ru(X)(Y)(R5R6PCHR1CR3R4CHR2PR7R8)(R9R10NCR13R14-Z-CR15R16NR11R12) where X, Y and diphosphine are as above and chiral diamine is, e.g., daipen (1-isopropyl-2,2-bis(p-methoxyphenyl)ethylenediamine). A process for enantioselectively preparing an alc. is provided whereby a carbonyl compound is reduced with H2 in the presence of 1 as catalyst. This asym. hydrogenation process has excellent results in terms of reactivity and enantioselectivity when compared with conventional Ru catalysts having an optically active diphosphine compound having the axial chirality or the asymmetry on C as the ligand. Thus, [RuBr2{(S,S)-Tolskewphos}{(R)-daipen}] [2, Tolskewphos = 2,4-bis(di-4-tolylphosphino)pentane] was prepared via [Ru{(S,S)-Tolskewphos}{methylallyl}] and [RuBr2{(S,S)-Tolskewphos}] intermediates. Asym. hydrogenation of acetophenone catalyzed by 2 in 2-propanol with added KOtMe3 as base afforded (R)-phenethyl alc. in ≥99% yield and 93.8% e.e.

- IC ICM C07F015-00
ICS C07C029-145; C07C029-14
- CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 21
- IT **Asymmetric synthesis and induction**
(enantioselective hydrogenation of carbonyl compds. to alcs. catalyzed by optically active ruthenium diphosphine complexes)
- IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective hydrogenation of carbonyl compds. to alcs. catalyzed by optically active ruthenium diphosphine complexes)
- IT 551950-95-9 551950-96-0
RL: CAT (Catalyst use); USES (Uses)
(asym. hydrogenation of carbonyl compds. to alcs. catalyzed by optically active ruthenium diphosphine complexes)
- IT 329735-86-6 329736-05-2 551950-89-1
552289-74-4
RL: CAT (Catalyst use); USES (Uses)
(optically active catalyst for asym. hydrogenation of carbonyl compds. to alcs.)
- IT 551950-86-8P 551950-90-4P 551950-94-8P
552289-81-3P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as optically active catalyst for asym. hydrogenation of carbonyl compds. to alcs.)
- IT 551950-88-0P 551950-93-7P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, coordinative addition of chiral diamine, and optically active catalyst for asym. hydrogenation of carbonyl compds. to alcs.)

L133 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:707996 CAPLUS Full-text

DOCUMENT NUMBER: 139:307568

TITLE: Rapid racemization of chiral non-racemic sec-alcohols catalyzed by (η⁵-C₅(CH₃)₅)Ru complexes bearing tertiary phosphine-primary amine chelate ligands

AUTHOR(S): Ito, Masato; Osaku, Akihide; Kitahara, Sachiko; Hirakawa, Makoto; Ikariya, Takao

CORPORATE SOURCE: Tokyo Institute of Technology, Frontier Collaborative Research Center, Department of Applied Chemistry, Graduate School of Science and Engineering, Meguro-ku, Tokyo, 152-8552, Japan

SOURCE: Tetrahedron Letters (2003), 44(40), 7521-7523
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:307568

ED Entered STN: 10 Sep 2003

AB A ternary catalyst system of chloro[(1,2,5,6- η)-1,5-cyclooctadiene][(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]ruthenium, 2-(diphenylphosphino)ethanamine and potassium tert-butoxide causes rapid racemization of chiral non-racemic sec-alcs., which results from the reversible hydrogen transfer between sec-alcs. and ketones. Other ligands thus screened included N,N-dimethyl-1,2-ethanediamine, 2-(diphenylphosphino)-N-methylethanamine, 2-(diphenylphosphino)-N,N-dimethylethanamine, 2-(phenylthio)ethanamine, 3-(diphenylphosphino)-1-propanamine, 2-(diphenylphosphino)benzenemethanamine. Both tertiary phosphine and primary amine functionalities in the ligand are responsible for the high rate. The role of solvents in this reaction was examined; the reaction of (α R)- α -methylbenzenemethanol in acetone as solvent yielded acetophenone, instead of (\pm)- α -methylbenzenemethanol, suggesting the intermediate formation of ketones. Isotope labeling expts. were also reported. In view of recent advances in dynamic kinetic resolution of racemic secondary alcs. in which the transition metal-catalyzed racemization is coupled with an enzymic transformation of alcs., the above catalyst system may also contribute to the dynamic kinetic resolution, since it exhibits a high catalyst performance under conditions favorable for enzymic reactions.

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Resolution (separation)
(kinetic, dynamic kinetic resolution;
racemization of chiral sec-alcs. catalyzed by
chloro[cyclooctadiene][pentamethylcyclopentadienyl]ruthenium/(diphenylphosphino)ethanamine in presence of potassium tert-butoxide)

IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(secondary, racemic secondary alcs.; racemization of chiral sec-alcs.
catalyzed by chloro[cyclooctadiene][pentamethylcyclopentadienyl]ruthenium/(diphenylphosphino)ethanamine in presence of potassium tert-butoxide)

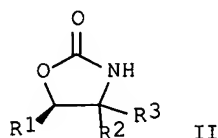
IT 108-00-9, N,N-Dimethyl-1,2-ethanediamine 865-47-4 2014-75-7,
2-(Phenylthio)ethanamine 4848-43-5, 2-(Diphenylphosphino)ethanamine
16605-03-1, 3-(Diphenylphosphino)-1-propanamine 29679-67-2,
2-(Diphenylphosphino)-N,N-dimethylethanamine 92390-26-6,
Chloro[(1,2,5,6- η)-1,5-cyclooctadiene][(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]ruthenium 177263-77-3,
2-(Diphenylphosphino)benzenemethanamine 350021-81-7,
2-(Diphenylphosphino)-N-methylethanamine
RL: CAT (Catalyst use); USES (Uses)
(racemization of chiral sec-alcs. catalyzed by
chloro[cyclooctadiene][pentamethylcyclopentadienyl]ruthenium/(diphenylphosphino)ethanamine in presence of potassium tert-butoxide)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 35 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:110336 CAPLUS Full-text

DOCUMENT NUMBER: 138:287562
 TITLE: Asymmetric Synthesis of Highly Substituted
 β -Nitro Alcohols and Enantiomerically Enriched
 4,4,5-Trisubstituted Oxazolidinones
 AUTHOR(S): Crich, David; Ranganathan, Krishnakumar; Rumthao,
 Sochanchingwung; Shirai, Michio
 CORPORATE SOURCE: Department of Chemistry, University of Illinois at
 Chicago, Chicago, IL, 60607-7061, USA
 SOURCE: Journal of Organic Chemistry (2003), 68(5), 2034-2037
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:287562
 ED Entered STN: 13 Feb 2003
 GI



- AB Asym. reduction of α,α -disubstituted- α -nitroketones $R_1COC(NO_2)R_2R_3$ [R_1 = Me, Et, $PhCH_2CH_2$, cyclohexyl, 2-furyl, 2-thienyl, R_2 = R_3 = Me; R_1 = $PhCH_2CH_2$, R_2R_3 = $(CH_2)_4$] with chiral oxazaborolidine, prepared in situ from $BH_3 \cdot Me_2S$ and (S)- α,α -diphenyl-2-pyrrolidinemethanol gave the corresponding trisubstituted nitro alcs. $R_1CH(OH)C(NO_2)R_2R_3$ (I) in good to excellent yields (49-94%) and with high enantiomeric excess. Reduction of I with Raney nickel to the corresponding amino alcs. and subsequent reaction of the latter with phosgene under basic conditions afforded enantiomerically enriched 4,4,5-trisubstituted oxazolidinones II.
- CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 23
- ST ketone nitro **enantioselective** redn; alc nitro asym synthesis
 redn; oxazolidinone trisubstituted asym synthesis
- IT **Alcohols, preparation**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (aliphatic, nitro; asym. synthesis of β -nitro alcs. and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β -nitro alcs., and chiral pyrrolidinemethanol-catalyzed reduction of β -nitro ketones)
- IT **Asymmetric synthesis and induction**
 (asym. synthesis of β -nitro alcs. and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β -nitro alcs., and chiral pyrrolidinemethanol-catalyzed reduction of β -nitro ketones)
- IT **Ketones, preparation**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (nitro; asym. synthesis of β -nitro alcs. and trisubstituted oxazolidinones via Henry reaction of aldehydes with

nitroalkanes, oxidation of racemic β -nitro alcs.,
and chiral pyrrolidinemethanol-catalyzed reduction of
 β -nitro ketones)

IT Reduction

Reduction catalysts

(stereoselective; asym. synthesis of β -nitro alcs. and
trisubstituted oxazolidinones via Henry reaction of aldehydes with
nitroalkanes, oxidation of racemic β -nitro alcs., and
chiral pyrrolidinemethanol-catalyzed reduction of β -nitro
ketones)

IT 75-07-0, Acetaldehyde, reactions 79-46-9, 2-Nitropropane 98-01-1,
2-Furancarboxaldehyde, reactions 98-03-3, 2-Thiophenecarboxaldehyde
104-53-0, 3-Phenylpropanal 123-38-6, Propanal, reactions 2043-61-0,
Cyclohexanecarboxaldehyde 2562-38-1, Nitrocyclopentane 20445-31-2,
(R)-MTPA

RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. synthesis of β -nitro alcs. and trisubstituted
oxazolidinones via Henry reaction of aldehydes with nitroalkanes,
oxidation of racemic β -nitro alcs., and chiral
pyrrolidinemethanol-catalyzed reduction of β -nitro ketones)

IT 13292-96-1P, 3-Methyl-3-nitro-2-butanone 20570-67-6P 20575-38-6P,
3-Methyl-3-nitro-2-butanol 32475-97-1P 82416-40-8P 85814-67-1P
89449-83-2P 101210-96-2P 504410-60-0P 504410-61-1P 504410-62-2P
504410-63-3P 504410-64-4P 504410-65-5P 504410-66-6P 504410-67-7P
504410-68-8P 504410-69-9P 504410-70-2P 504410-71-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(asym. synthesis of β -nitro alcs. and trisubstituted
oxazolidinones via Henry reaction of aldehydes with nitroalkanes,
oxidation of racemic β -nitro alcs., and chiral
pyrrolidinemethanol-catalyzed reduction of β -nitro ketones)

IT 154278-27-0P 159090-84-3P 504410-72-4P 504410-73-5P 504410-74-6P
504410-75-7P 504410-76-8P 504410-77-9P 504410-78-0P 504410-79-1P
504410-80-4P 504410-81-5P 504410-82-6P 504410-83-7P 504410-84-8P
504410-85-9P 504410-86-0P 504410-87-1P 504410-88-2P 504410-89-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(asym. synthesis of β -nitro alcs. and trisubstituted
oxazolidinones via Henry reaction of aldehydes with nitroalkanes,
oxidation of racemic β -nitro alcs., and chiral
pyrrolidinemethanol-catalyzed reduction of β -nitro ketones)

IT 112068-01-6, (S)- α,α -Diphenyl-2-pyrrolidinemethanol

RL: CAT (Catalyst use); USES (Uses)

(reduction catalyst; asym. synthesis of β -nitro alcs. and
trisubstituted oxazolidinones via Henry reaction of aldehydes with
nitroalkanes, oxidation of racemic β -nitro alcs., and
chiral pyrrolidinemethanol-catalyzed reduction of β -nitro
ketones)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 36 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:525760 CAPLUS Full-text

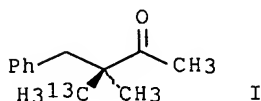
DOCUMENT NUMBER: 137:216470

TITLE: Isotopically Chiral Probes for in Situ High-Throughput
Asymmetric Reaction Analysis

AUTHOR(S): Evans, Michael A.; Morken, James P.

CORPORATE SOURCE: Department of Chemistry, Venable and Kenan

SOURCE: Laboratories, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-3290, USA
 Journal of the American Chemical Society (2002), 124(31), 9020-9021
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:216470
 ED Entered STN: 16 Jul 2002
 GI



- AB A nonracemic 13C-labeled ketone I was prepared and used as a chiral probe in a high-throughput screening assay for ligands in ruthenium-catalyzed asym. transfer hydrogenation. I is nonracemic because of the presence of the isotopic label, but because the enantiomers differ very little in their steric environments, I exhibits chemical behavior similar to an achiral ketone in asym. reactions. The products of asym. reactions of I are diastereomers by virtue of the isotopic carbon labels. The carbon labels in products derived from asym. transformations of I are in diastereotopic environments and therefore lead to unique NMR resonances; the presence of a 13C isotopic label allows for rapid anal. of the diastereomers by 13C NMR. The effective "enantiomeric excess" of the reaction is determined through the use of single pulse, nonspinning, unlocked, and unshimmed 13C NMR spectroscopy; integration of the peaks for the diastereomers and calcn. of the ratio of diastereomers gives an estimate of the enantiomer excesses and conversions of the corresponding reaction with the analogous achiral ketone PHCH₂CMe₂COMe. Chiral GC anal. of reactions performed with I gave measurements of the diastereomeric excesses similar to those obtained using 13C NMR. The anal. of a single reaction by this technique can be performed in approx. 15 s. I was used as a chiral probe mol. in the asym. transfer hydrogenation of ketones in the presence of ruthenium arene complexes and amino alcs. Simple amino alcs. such as (R)- and (S)-phenylglycinol and a bis(η⁶-hexamethylbenzene)ruthenium dichloride precursor were found to generate the most effective catalysts in asym. transfer hydrogenation of I. The use of (R)- and (S)-phenylglycinol as catalysts for the asym. transfer hydrogenation reactions of acetophenone and 3-methyl-2-butanone with bis(η⁶-hexamethylbenzene)ruthenium dichloride) with isopropanol and potassium hydroxide gave the corresponding secondary alcs. in 22-64% ee and in 92-98% conversions.
- CC 21-2 (General Organic Chemistry)
- ST carbon 13 labeled ketone prepn chiral probe asym reaction; high throughput screening carbon 13 labeled ketone chiral probe; screening ruthenium amino alc catalyst asym hydrogenation ketone
- IT Alcohols, uses
 RL: CAT (Catalyst use); USES (Uses)
 (amino; high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C

- NMR-based assay)
- IT NMR (nuclear magnetic resonance)
(carbon-13; high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C NMR-based assay)
- IT Asymmetric synthesis and induction
(preparation of a nonracemic 13C-labeled ketone as a chiral probe for use in a 13C NMR-based method for the high-throughput screening of catalysts for asym. reactions)
- IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(secondary; enantioselective preparation of secondary alcs. by asym. transfer hydrogenation of ketones in the presence of ruthenium complexes of amino alcs.)
- IT Hydrogenation
Hydrogenation catalysts
(transfer, stereoselective; high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C NMR-based assay)
- IT 90-82-4, (+)-Pseudoephedrine 147-85-3, L-Proline, uses 7531-52-4, (S)-Prolinamide 20989-17-7, (S)-Phenylglycinol 37366-09-9 51594-34-4 52462-29-0 56613-80-0, (R)-Phenylglycinol 67421-02-7 68832-13-3, (R)-Prolinol 71581-92-5 79815-20-6 163061-74-3, (1S,2S)-1-Amino-2-indanol
RL: CAT (Catalyst use); USES (Uses)
(high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C NMR-based assay)
- IT 457064-02-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C NMR-based assay)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 37 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:880431 CAPLUS Full-text

DOCUMENT NUMBER: 138:106546

TITLE: Chemoenzymatic Dynamic Kinetic Resolution of β -Halo Alcohols. An Efficient Route to Chiral Epoxides

AUTHOR(S): Pamies, Oscar; Baekvall, Jan-E.

CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, SE-10691, Swed.

SOURCE: Journal of Organic Chemistry (2002), 67(25), 9006-9010
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:106546

ED Entered STN: 21 Nov 2002

AB Enzymic resolution of β -chloro alcs. in combination with ruthenium-catalyzed alc. isomerization led to a successful dynamic kinetic resolution (conversion up to 99% and ee up to 97%). The efficiency of the DKR is dramatically

reduced when β -bromo alcs. are used. The presence of the bromo substituent causes decomposition of the ruthenium catalysts, which triggers the progressive deactivation of the enzyme. The synthetic utility of this procedure has been illustrated by the practical synthesis of different chiral epoxides.

CC 27-2 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 23

IT Resolution (separation)

(enzymic, kinetic; chemoenzymic dynamic kinetic resolution of β -halo alcs. and subsequent conversion of intermediate acetates to chiral epoxides)

IT Alcohols, preparation

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(halo, β -; chemoenzymic dynamic kinetic resolution of β -halo alcs. and subsequent conversion of intermediate acetates to chiral epoxides)

IT Resolution (separation)

(kinetic, dynamic; chemoenzymic dynamic kinetic resolution of β -halo alcs. and subsequent conversion of intermediate acetates to chiral epoxides)

IT 104439-77-2

RL: CAT (Catalyst use); USES (Uses)

(racemization catalyst; chemoenzymic dynamic kinetic resolution of β -halo alcs. and subsequent conversion of intermediate acetates to chiral epoxides)

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:550664 CAPLUS Full-text

DOCUMENT NUMBER: 138:39057

TITLE: Fine-tuning of modular amino alcohol ligands for the enantioselective transfer hydrogenation of ketones

AUTHOR(S): Pasto, Mireia; Riera, Antoni; Pericas, Miquel A.

CORPORATE SOURCE: Unitat de Recerca en Sintesi Asimetrica (URSA-PCB), Departament de Quimica Organica / Parc Cientific de Barcelona, Universitat de Barcelona, Barcelona, 08028, Spain

SOURCE: European Journal of Organic Chemistry (2002), (14), 2337-2341

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:39057

ED Entered STN: 25 Jul 2002

AB A family of stereodefined, modular amino alcs. (3-alkoxy-1-amino-1-phenyl- 2-propanols), in which the steric bulk of the alkoxy and amino substituents varies smoothly, has been synthesized from enantiomerically pure phenylglycidol, prepared by Sharpless epoxidn. These amino alcs. have been evaluated as ligands in the catalyzed [(amino alc.)(arene)RuII] transfer hydrogenation of alkyl aryl ketones with 2-propanol as the hydrogen source. Both the nitrogen substituent and the alkoxy group have been optimized for maximal enantioselectivity and catalytic activity in the process under consideration.

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Alcohols, preparation

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP

(Preparation); USES (Uses)

(amino, aromatic; amino alc.-ruthenium complex catalysts for asym. transfer hydrogenation of acetophenone to (S)- α -methylbenzyl alc.)

IT 52462-29-0

RL: CAT (Catalyst use); USES (Uses)

(amino alc.-ruthenium complex catalysts for asym. transfer hydrogenation of acetophenone to (S)- α -methylbenzyl alc.)

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 39 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:751983 CAPLUS Full-text

DOCUMENT NUMBER: 136:247366

TITLE: The first Ru(II)-catalysed asymmetric hydrogen transfer reduction of aromatic ketones in aqueous media

AUTHOR(S): Rhyoo, Hae Yoon; Park, Hee-Jung; Chung, Young Keun
CORPORATE SOURCE: School of Chemistry and Center for Molecular Catalysis, Seoul National University, Seoul, 151-747, S. Korea

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (20), 2064-2065
CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:247366

ED Entered STN: 15 Oct 2001

AB The first water-soluble asym. H-transfer Ru(II) catalyst system consisting of [Ru(p-cymene)Cl₂]₂, (S)-proline amide, and HCOONa, which gives high conversion rates with high ee values up to 95.3% and is reusable, was developed.

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Alcohols, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(aralkyl; enantioselective preparation by asym. hydrogen transfer reduction

of

aromatic ketones using (S)-proline amide and ruthenium(II) catalysts in aqueous media)

IT 52462-29-0 64030-43-9 84846-34-4 367521-34-4

RL: CAT (Catalyst use); USES (Uses)

(enantioselective preparation of aromatic alcs. by asym. hydrogen transfer reduction of aromatic ketones using (S)-proline amide and ruthenium(II) catalysts in aqueous media)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:471574 CAPLUS Full-text

DOCUMENT NUMBER: 133:237617

TITLE: A catalytic enantioselective allylation reaction of aldehydes in an aqueous medium

AUTHOR(S): Loh, T.-P.; Zhou, J.-R.
CORPORATE SOURCE: Department of Chemistry, National University of Singapore, Singapore, 117543, Singapore

SOURCE: Tetrahedron Letters (2000), 41(27), 5261-5264
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:237617

ED Entered STN: 13 Jul 2000

AB A modified Yamamoto-Yanagisawa's catalyst (S)-Tol-BINAP·AgNO₃ was successfully applied to a catalytic enantioselective allylation reaction of aldehydes in an aqueous system. The reactions with aromatic aldehydes afforded the desired products in high yields with good stereoselectivities. E.g., (S)-Tol-BINAP·AgNO₃ (0.1 mmol) was treated with 1-naphthaldehyde (1 mmol) and allyltributyltin (1 mmol) in the dark with stirring, affording the corresponding allyl alc. in quant. yield and 81% ee.

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Alcohols, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(allyl; enantioselective allylation reaction of aromatic aldehydes in aqueous

medium, catalyzed by modified Yamamoto-Yanagisawa's catalyst)

IT 2923-28-6, Silver triflate 7761-88-8, Silver nitrate, uses 7783-92-8, Silver chloride 10102-05-3, Palladium dinitrate 20759-14-2 21797-13-7 35658-65-2 42196-31-6 64443-05-6

RL: CAT (Catalyst use); USES (Uses)

(in situ formation with chiral diphosphines of catalyst for enantioselective allylation reaction of aromatic aldehydes)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 41 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:756096 CAPLUS Full-text

DOCUMENT NUMBER: 134:43672

TITLE: Asymmetric activation/deactivation of racemic Ru catalysts for highly enantioselective hydrogenation of ketonic substrates

AUTHOR(S): Mikami, Koichi; Korenaga, Toshinobu; Ohkuma, Takeshi; Noyori, Ryoji

CORPORATE SOURCE: Dep. Chemical Technology, Tokyo Institute Technology, Tokyo, 152-8552, Japan

SOURCE: Angewandte Chemie, International Edition (2000), 39(20), 3707-3710
CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 27 Oct 2000

AB An asym. activation/ deactivation strategy was developed for highly enantioselective hydrogenation irresp. of the ketonic substrates used by maximizing the difference in the catalytic activity between the enantiomeric catalysts. Thus, the present asym. activation/ deactivation protocol can be regarded as a paradigm shift in racemic catalysis.

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 67, 75, 78

IT Bond angle

Bond length

Hydrogenation catalysts

(asym. activation/deactivation of racemic Ru catalysts for highly enantioselective hydrogenation of ketonic substrates)

IT Ketones, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. activation/deactivation of racemic Ru catalysts for highly enantioselective hydrogenation of ketonic substrates)

IT Alcohols, preparation

RL: IMF (Industrial manufacture); PREP (Preparation)

(asym.; asym. activation/deactivation of racemic Ru catalysts for

highly enantioselective hydrogenation of ketonic substrates)

IT Crystal structure
Molecular structure
(of asym. racemic Ru catalysts for highly enantioselective hydrogenation of ketonic substrates)

IT 78-59-1, Isophorone 93-08-3, Methyl 2-naphthyl ketone 98-86-2, Acetophenone, reactions 122-00-9 577-16-2 585-74-0 941-98-0, Methyl 1-naphthyl ketone
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. activation/deactivation of racemic Ru catalysts for highly enantioselective hydrogenation of ketonic substrates)

IT 29841-69-8, (S,S)-1,2-Diphenylethylenediamine 35132-20-8, (R,R)-1,2-Diphenylethylenediamine 312969-46-3
RL: CAT (Catalyst use); USES (Uses)
(catalyst activator; asym. activation/deactivation of racemic Ru catalysts for highly enantioselective hydrogenation of ketonic substrates)

IT 42177-25-3, (R)-1-(1-Naphthyl)ethanol
RL: CAT (Catalyst use); USES (Uses)
(catalyst; asym. activation/deactivation of racemic Ru catalysts for highly enantioselective hydrogenation of ketonic substrates)

IT 115245-70-0
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(catalyst; asym. activation/deactivation of racemic Ru catalysts for highly enantioselective hydrogenation of ketonic substrates)

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 42 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:3672 CAPLUS Full-text
DOCUMENT NUMBER: 80:3672
TITLE: Optically active secondary alcohols
INVENTOR(S): Solodar, Arthur J.
PATENT ASSIGNEE(S): Monsanto Co.
SOURCE: Ger. Offen., 33 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
DE 2312924	A1	19730927	DE 1973-2312924	19730315
FR 2176128	A1	19731026	FR 1973-9394	19730315
JP 49001505	A	19740108	JP 1973-29547	19730315
GB 1423911	A	19760204	GB 1973-12510	19730315
CA 1000293	A1	19761123	CA 1973-166348	19730315
CH 593217	A5	19771130	CH 1973-3760	19730315
PRIORITY APPLN. INFO.:			US 1972-235405	A 19720316

ED Entered STN: 12 May 1984

AB Optically active secondary alcs., e.g. d- and l-menthol (I), ephedrine, pseudoephedrine, and threo- and erythro-AcNHCHMeCHPhOH, were prepared without any addnl. separation step by hydrogenation of the racemic ketones in the presence of coordination compds. of Rh with optically active phosphine ligands, e.g. bis(cyclohexyl-methyl-o-anisylphosphine)-1,5-cyclooctadienerhodium tetrafluoroborate (II). Thus, (±)-menthone was hydrogenated over optically active II in H₂O-Me₂CHCO₂H 9.5 hr at 72° and 5.9

kg/cm² to give menthol of optical purity 29.2% and which contained preponderantly I.

IC C07B; C07C; B01J

CC 30-10 (Terpenoids)

Section cross-reference(s): 63, 25, 34

IT Ketones, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrogenation of racemic, optically active alcs. by)

IT Asymmetric synthesis and induction

(of alcs., by hydrogenation of racemic ketones in presence of rhodium phosphine complexes)

IT Alcohols, preparation

RL: PREP (Preparation)

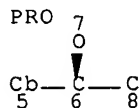
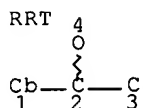
(optically active, by hydrogenation of racemic ketones)

FILE 'HOME' ENTERED AT 16:47:51 ON 02 FEB 2007

SEARCH HISTORY

=> d stat que l125

L14 152839 SEA FILE=REGISTRY ABB=ON RU/ELS
 L24 1 SEA FILE=REGISTRY ABB=ON SUBTILISIN/CN
 L25 1 SEA FILE=REGISTRY ABB=ON PROTEINASE/CN
 L67 72677 SEA FILE=CASREACT ABB=ON STEREOSELECTIVE/NTE
 L68 30236 SEA FILE=REGISTRY ABB=ON L14 AND CASREACT/LC
 L69 8227 SEA FILE=CASREACT ABB=ON L68/CAT
 L70 267 SEA FILE=CASREACT ABB=ON L24/CAT OR L25/CAT
 L73 76833 SEA FILE=CASREACT ABB=ON (L69 OR L70 OR L67)
 L76 STR



NODE ATTRIBUTES:

CONNECT IS E3 RC AT 2
 CONNECT IS E1 RC AT 4
 CONNECT IS E3 RC AT 6
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 1
 GGCAT IS UNS AT 5
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES:

STEREO DEFAULT ABSOLUTE
 NUMBER OF CHIRAL CENTERS IS 1

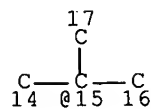
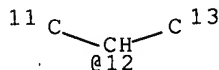
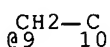
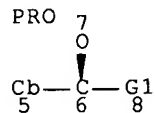
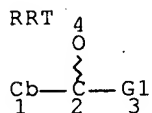
****MAPPINGS****

NOD SYM	ROL	NOD SYM	ROL
2 C	RRT	6 C	PRO
4 O	RRT	7 O	PRO
6 C	PRO	2 C	RRT
7 O	PRO	4 O	RRT

L82 SCR 1149

L87 3195 SEA FILE=CASREACT SUB=L73 SSS FUL L76 AND L82 (20816 REACTIONS)

L122 STR



VAR G1=CH3/9/12/15

NODE ATTRIBUTES:

CONNECT IS E3 RC AT 2
 CONNECT IS E1 RC AT 4

CONNECT IS E3 RC AT 6
 DEFAULT MLEVEL IS ATOM
 GGCAT IS UNS AT 1
 GGCAT IS UNS AT 5
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 17

STEREO ATTRIBUTES:
 STEREO DEFAULT ABSOLUTE
 NUMBER OF CHIRAL CENTERS IS 1

****MAPPINGS****

NOD	SYM	ROL	NOD	SYM	ROL
2	C	RRT	6	C	PRO
4	O	RRT	7	O	PRO
6	C	PRO	2	C	RRT
7	O	PRO	4	O	RRT

L124 1785 SEA FILE=CASREACT SUB=L87 SSS FUL L122 (10785 REACTIONS)
 L125 1783 SEA FILE=CASREACT ABB=ON L124/COMPLETE

=> d his nofile

(FILE 'HOME' ENTERED AT 09:49:53 ON 02 FEB 2007)

FILE 'REGISTRY' ENTERED AT 09:50:16 ON 02 FEB 2007

D SAVED
 ACT CHO829REG/A

L1 59 SEA ABB=ON (104439-77-2/BI OR 108-21-4/BI OR 108-82-7/BI OR
 108-88-3/BI OR 109-99-9/BI OR 117636-42-7/BI OR 1193-81-3/BI
 OR 123-91-1/BI OR 123-96-6/BI OR 13991-52-1/BI OR 1445-91-6/BI
 OR 1517-68-6/BI OR 151716-02-8/BI OR 1572-97-0/BI OR 161024-76-
 6/BI OR 16197-93-6/BI OR 219119-78-5/BI OR 219119-82-1/BI OR
 221911-67-7/BI OR 25501-32-0/BI OR 3113-98-2/BI OR 3319-15-1/BI
 OR 3391-10-4/BI OR 371-27-7/BI OR 406-95-1/BI OR 470688-18-7/B
 I OR 52462-29-0/BI OR 529-34-0/BI OR 53732-47-1/BI OR 56-23-5/B
 I OR 5876-76-6/BI OR 600-36-2/BI OR 6169-06-8/BI OR 617713-61-8
 /BI OR 617713-62-9/BI OR 617713-63-0/BI OR 6351-10-6/BI OR
 6398-51-2/BI OR 64-18-6/BI OR 67-66-3/BI OR 698-87-3/BI OR
 701-70-2/BI OR 71-43-2/BI OR 7376-05-8/BI OR 7476-81-5/BI OR
 75-09-2/BI OR 835893-52-2/BI OR 835893-53-3/BI OR 835893-54-4/B
 I OR 835893-55-5/BI OR 835893-56-6/BI OR 837424-43-8/BI OR
 9001-73-4/BI OR 9001-92-7/BI OR 9004-07-3/BI OR 9014-01-1/BI
 OR 98-85-1/BI OR 99528-42-4/BI OR 99897-61-7/BI)

 D SCAN

FILE 'STNGUIDE' ENTERED AT 09:50:50 ON 02 FEB 2007

FILE 'LREGISTRY' ENTERED AT 09:51:46 ON 02 FEB 2007

E S/CN
 E (S)/CN

L2 1 SEA ABB=ON "(S)-(+) -1-BUTEN-3-OL"/CN
 D IDE
 L3 STR 6118-13-4
 L4 STR

L5 0 SEA SSS SAM L4
 L6 15 SEA SSS FUL L4
 D SCAN
 L7 STR L4
 L8 STR L7
 L9 0 SEA SSS SAM L8
 L10 33 SEA SSS FUL L8
 L11 18 SEA ABB=ON L10 NOT L6
 D SCAN L6
 D SCAN
 D SET

FILE 'CASREACT' ENTERED AT 12:25:45 ON 02 FEB 2007

L12 STR
 L13 13 SEA SSS SAM L12 (101 REACTIONS)

FILE 'REGISTRY' ENTERED AT 12:29:16 ON 02 FEB 2007

L14 152839 SEA ABB=ON RU/ELS

FILE 'CAPLUS' ENTERED AT 12:29:24 ON 02 FEB 2007

L15 101120 SEA ABB=ON L14
 L16 25439 SEA ABB=ON L15(L)CAT/RL
 L17 150091 SEA ABB=ON ALCOHOLS/CT
 L18 0 SEA ABB=ON L17(L)PREP/CT
 L19 18354 SEA ABB=ON L17(L)PREP/RL
 L20 136 SEA ABB=ON L19(L)"S"/OBI

FILE 'STNGUIDE' ENTERED AT 12:33:39 ON 02 FEB 2007

FILE 'CAPLUS' ENTERED AT 12:36:02 ON 02 FEB 2007

E ASYMMETRIC SYNTHESIS AND INDUCTION+ALL/CT
 L21 33996 SEA ABB=ON "ASYMMETRIC SYNTHESIS AND INDUCTION"+OLD,NT/CT
 E RESOLUTION/CT
 E E11+ALL
 L22 23387 SEA ABB=ON "RESOLUTION (SEPARATION)+"OLD/CT
 L23 6 SEA ABB=ON L16 AND L20
 D SCAN TI
 SAVE TEMP L23 CHO829CA1/A

FILE 'REGISTRY' ENTERED AT 12:39:28 ON 02 FEB 2007

L24 1 SEA ABB=ON SUBTILISIN/CN
 L25 1 SEA ABB=ON PROTEINASE/CN

FILE 'CAPLUS' ENTERED AT 12:39:38 ON 02 FEB 2007

L26 51371 SEA ABB=ON (L24 OR L25)
 L27 2353 SEA ABB=ON L26(L)CAT/RL
 L28 995 SEA ABB=ON DYNAMIC/OBI(L)KINETIC/OBI
 L29 226 SEA ABB=ON L28(L)L22
 L30 9 SEA ABB=ON L29 AND (L16 OR L27) AND L19
 SAVE TEMP L30 CHO820CA2/A
 D QUE L23
 L31 6 SEA ABB=ON L20 AND (L16 OR L27)
 SAVE TEMP L31 CHO829CA1/A
 L32 145 SEA ABB=ON L19 AND L21 AND (L27 OR L16)
 L33 1746 SEA ABB=ON ACHIRAL/OBI
 L34 4 SEA ABB=ON L32 AND L33
 D SCAN
 L35 3653 SEA ABB=ON CHIRAL/OBI(L) (ALCOHOL/OBI OR ALCS/OBI)
 D QUE L32
 L36 61 SEA ABB=ON L19 AND L35 AND L21 AND (L27 OR L16)

L37 2 SEA ABB=ON L19 AND L35 AND L21 AND (L27 OR L16) AND L33
 SAVE TEMP L37 CHO829CA3/A
 D QUE L30
 D QUE L31
 D QUE L37
 L38 5627 SEA ABB=ON ACHIRAL/BI
 L39 3 SEA ABB=ON L19 AND L35 AND L21 AND (L27 OR L16) AND L38
 L40 1 SEA ABB=ON L39 NOT L37
 D SCAN
 L41 19466 SEA ABB=ON ENANTIOSELECT?/OBI
 L42 4 SEA ABB=ON L19(L)L41 AND L35 AND L21 AND (L27 OR L16)
 D SCAN TI
 SAVE TEMP L39 CHO829CA3/A
 SAVE TEMP L42 CHO829CA4/A
 L43 66509 SEA ABB=ON KETONES/CT
 L44 11738 SEA ABB=ON RACEMIC/OBI
 L45 10 SEA ABB=ON L43(L)L44 AND L19 AND (L20 OR L21 OR L22 OR L35 OR
 L41)
 SAVE TEMP L45 CHO829CA5/A

FILE 'CASREACT' ENTERED AT 12:52:19 ON 02 FEB 2007

D QUE L12
 L46 13 SEA SSS SAM L12 (101 REACTIONS)
 D SCAN

FILE 'LCASREACT' ENTERED AT 14:49:38 ON 02 FEB 2007

E A/NTE
 E STER/NTE
 E A/NTE
 L47 2 SEA ABB=ON TUBE/NTE
 D IBIB ABS FHIT
 D IBIB ABS HIT
 L48 STR L12
 L49 3 SEA SSS SAM L48 (8 REACTIONS)
 D IALL
 D HIT
 D HIT 2-3
 E STEREOSELECT?
 L50 64 SEA ABB=ON STEREOS?
 D HIT 1-10
 D IT 1-15
 L51 STR L48
 L52 0 SEA SSS SAM L51 (0 REACTIONS)
 L53 8 SEA SSS FUL L51 (48 REACTIONS)
 D FHIT 1-8
 L54 45 SEA ABB=ON STEREOCHEMISTRY/CT
 L55 14 SEA ABB=ON ASYMMETRIC/CW
 D HIT
 L56 3 SEA ABB=ON L53 AND (L50 OR L54 OR L55)
 D HIT 1-3
 L57 STR L51
 L58 3 SEA SSS SAM L57 (8 REACTIONS)
 D SCAN
 D FHIT 1-3

FILE 'CASREACT' ENTERED AT 15:14:56 ON 02 FEB 2007

L59 335 SEA ABB=ON KIM M?/AU
 L60 448 SEA ABB=ON PARK J?/AU
 L61 212 SEA ABB=ON CHUNG Y?/AU
 L62 255 SEA ABB=ON CHOI J?/AU

L63 702 SEA ABB=ON LEE H?/AU
 L64 126 SEA ABB=ON CHOI Y?/AU
 L65 530 SEA ABB=ON KIM D?/AU
 L66 1 SEA ABB=ON L59 AND L60 AND L61 AND L62 AND L63 AND L64 AND
 L65
 D SCAN
 D IALL

FILE 'STNGUIDE' ENTERED AT 15:16:21 ON 02 FEB 2007

FILE 'CASREACT' ENTERED AT 15:18:38 ON 02 FEB 2007
 E STER/NTE

L67 72677 SEA ABB=ON STEREOSELECTIVE/NTE

FILE 'REGISTRY' ENTERED AT 15:19:19 ON 02 FEB 2007
 L68 30236 SEA ABB=ON L14 AND CASREACT/LC

FILE 'CASREACT' ENTERED AT 15:20:32 ON 02 FEB 2007

FILE 'REGISTRY' ENTERED AT 15:21:01 ON 02 FEB 2007

FILE 'CASREACT' ENTERED AT 15:21:57 ON 02 FEB 2007
 L69 8227 SEA ABB=ON L68/CAT
 L70 267 SEA ABB=ON L24/CAT OR L25/CAT
 D QUE L57
 L71 STR L57
 L72 12 SEA SSS SAM L71 (95 REACTIONS)
 L73 76833 SEA ABB=ON (L69 OR L70 OR L67)
 L74 23 SEA SUB=L73 SSS SAM L71 (169 REACTIONS)
 L75 4126 SEA SUB=L73 SSS FUL L71 (43895 REACTIONS)
 SAVE TEMP L75 CHO829CASRE/A

FILE 'STNGUIDE' ENTERED AT 15:26:18 ON 02 FEB 2007

FILE 'LREGISTRY' ENTERED AT 15:27:28 ON 02 FEB 2007

FILE 'STNGUIDE' ENTERED AT 15:33:25 ON 02 FEB 2007

FILE 'CASREACT' ENTERED AT 15:42:43 ON 02 FEB 2007

L76 STR L71
 L77 7 SEA SSS SAM L76 (71 REACTIONS)
 L78 11 SEA SUB=L73 SSS SAM L76 (94 REACTIONS)
 L79 STR L76
 L80 5 SEA SSS SAM L79 (44 REACTIONS)
 D SCAN
 E ANY/CAT
 L81 11 SEA SUB=L73 SSS SAM L76 (94 REACTIONS)
 L*** DEL SCREEN 1701
 L82 SCREEN 1149
 D QUE L77
 L83 11 SEA SUB=L73 SSS SAM L76 (94 REACTIONS)
 L84 24 SEA SSS SAM L76 AND L82 (178 REACTIONS)
 L85 13 SEA SUB=L73 SSS SAM L76 AND L82 (112 REACTIONS)
 D SCAN
 L86 13 SEA SUB=L73 SSS SAM L76 AND L82 (112 REACTIONS)
 L87 3195 SEA SUB=L73 SSS FUL L76 AND L82 (20816 REACTIONS)
 L88 3187 SEA ABB=ON L87/COMPLETE
 SAVE TEMP L88 CHO829CASRE/A
 L89 520 SEA ABB=ON L88 AND (L69 OR L70) AND L67
 L90 5 SEA ABB=ON L88 AND L69 AND L70 AND L67

L91 517 SEA ABB=ON (L59 OR L60 OR L61 OR L62 OR L63 OR L64 OR L65)
 AND L67
 L92 35 SEA ABB=ON (L59 OR L60 OR L61 OR L62 OR L63 OR L64 OR L65)
 AND L67 AND L88
 L93 19 SEA ABB=ON (L59 OR L60 OR L61 OR L62 OR L63 OR L64 OR L65)
 AND L67 AND L88 AND (L69 OR L70)
 L94 207 SEA ABB=ON (L59 AND (L60 OR L61 OR L62 OR L63 OR L64 OR L65))
 OR (L60 AND (L61 OR L62 OR L63 OR L64 OR L65)) OR (L61 AND
 (L62 OR L63 OR L64 OR L65)) OR (L62 AND (L63 OR L64 OR L65))
 OR (L63 AND (L64 OR L65)) OR (L64 AND L65)
 L95 13 SEA ABB=ON L94 AND L88 AND L67
 L96 14 SEA ABB=ON L94 AND L88 AND (L69 OR L70)
 L97 13 SEA ABB=ON L95 AND L96
 L98 3 SEA ABB=ON L90 AND L97
 D QUE NOS L90
 L99 STR L76
 L100 0 SEA SUB=L87 SSS SAM L99 (0 REACTIONS)
 L101 0 SEA SUB=L87 SSS FUL L99 (0 REACTIONS)
 L102 512 SEA ABB=ON L88 AND L69 AND L67
 L103 13 SEA ABB=ON L88 AND L70 AND L67
 E ENZYM/CAT
 E ENZYM/NTE
 L104 9228 SEA ABB=ON ENZYM?/NTE
 L105 28 SEA ABB=ON L102 AND L104

FILE 'CAPLUS' ENTERED AT 16:03:45 ON 02 FEB 2007

L106 14460 SEA ABB=ON KIM M?/AU
 L107 25330 SEA ABB=ON PARK J?/AU
 L108 4144 SEA ABB=ON CHUNG Y?/AU
 L109 11169 SEA ABB=ON CHOI J?/AU
 L110 29440 SEA ABB=ON LEE H?/AU
 L111 8289 SEA ABB=ON CHOI Y?/AU
 L112 23463 SEA ABB=ON KIM D?/AU
 L113 1 SEA ABB=ON L106 AND L107 AND L108 AND L109 AND L110 AND L111
 AND L112

FILE 'CASREACT' ENTERED AT 16:06:06 ON 02 FEB 2007

SAVE TEMP L97 CHO829CRAU/A
 SAVE TEMP L103 CHO829CR1/A
 SAVE TEMP L105 CHO829CR2/A

FILE 'CAPLUS' ENTERED AT 16:06:39 ON 02 FEB 2007

L114 8708 SEA ABB=ON (L106 AND (L107 OR L108 OR L109 OR L110 OR L111 OR
 L112)) OR (L107 AND (L108 OR L109 OR L110 OR L111 OR L112)) OR
 (L108 AND (L109 OR L110 OR L111 OR L112)) OR (L109 AND (L110
 OR L111 OR L112)) OR (L110 AND (L111 OR L112)) OR (L111 AND
 L112)
 L115 22 SEA ABB=ON L114 AND (L28 OR L35 OR L20)
 L116 17 SEA ABB=ON L114 AND (L29 OR L35 OR L20)
 D SCAN TI

FILE 'CAPLUS' ENTERED AT 16:09:57 ON 02 FEB 2007

D QUE L113
 D QUE L116
 L117 17 SEA ABB=ON (L113 OR L116)

FILE 'CASREACT' ENTERED AT 16:10:08 ON 02 FEB 2007
 D QUE NOS L97

FILE 'CASREACT, CAPLUS' ENTERED AT 16:10:19 ON 02 FEB 2007

L118 24 DUP REM L97 L117 (6 DUPLICATES REMOVED)
 ANSWERS '1-13' FROM FILE CASREACT
 ANSWERS '14-24' FROM FILE CAPLUS
 D IBIB ABS FHIT 1-13
 D IBIB ED ABS HITIND 14-24

FILE 'CASREACT' ENTERED AT 16:11:35 ON 02 FEB 2007
 D STAT QUE L88
 D QUE NOS L103
 D QUE NOS L105

L119 28 SEA ABB=ON (L103 OR L105) NOT L97

FILE 'CAPLUS' ENTERED AT 16:12:13 ON 02 FEB 2007
 D QUE L31
 D QUE L30
 D QUE L39
 D QUE L42
 D QUE L45

L120 27 SEA ABB=ON (L31 OR L30 OR L39 OR L42 OR L45) NOT L117

FILE 'CASREACT, CAPLUS' ENTERED AT 16:12:27 ON 02 FEB 2007

L121 52 DUP REM L119 L120 (3 DUPLICATES REMOVED)
 ANSWERS '1-28' FROM FILE CASREACT
 ANSWERS '29-52' FROM FILE CAPLUS
 D IBIB ABS FHIT 1-28
 D IBIB ED ABS HITIND 29-52

FILE 'HOME' ENTERED AT 16:13:35 ON 02 FEB. 2007
 D STAT QUE L88
 D SAVED

FILE 'CASREACT' ENTERED AT 16:38:39 ON 02 FEB 2007

D QUE L99
 D QUE L79
 D QUE NOS L88
 L122 STR L79
 L123 50 SEA SUB=L87 SSS SAM L122 (330 REACTIONS)
 L124 1785 SEA SUB=L87 SSS FUL L122 (10785 REACTIONS)
 L125 1783 SEA ABB=ON L124/COMPLETE
 SAVE TEMP L125 CH0829CRSUB/A
 D QUE NOS L103
 L126 5 SEA ABB=ON L125(L)L69(L)L70
 L127 363 SEA ABB=ON L125(L) (L69 OR L70) AND L67
 L128 350 SEA ABB=ON L125(L) (L69 OR L70) (L) L67
 D QUE NOS L105
 L129 9 SEA ABB=ON L125(L)L70
 L130 21 SEA ABB=ON L125(L)L69(L)L67(L)L104

FILE 'CASREACT' ENTERED AT 16:45:47 ON 02 FEB 2007

D STAT QUE L125
 D QUE NOS L129
 D QUE NOS L130
 L131 17 SEA ABB=ON (L129 OR L130) NOT L97

FILE 'CAPLUS' ENTERED AT 16:46:32 ON 02 FEB 2007

D QUE L31
 D QUE L30
 D QUE L39
 D QUE L42
 D QUE L45

L132 27 SEA ABB=ON (L31 OR L30 OR L39 OR L42 OR L45) NOT L117

FILE 'CASREACT, CAPLUS' ENTERED AT 16:46:51 ON 02 FEB 2007
L133 42 DUP REM L131 L132 (2 DUPLICATES REMOVED)
ANSWERS '1-17' FROM FILE CASREACT
ANSWERS '18-42' FROM FILE CAPLUS
D IBIB ABS FHIT
D IBIB ABS FHIT 2-17
D IBIB ED ABS HITIND 18-42

FILE 'HOME' ENTERED AT 16:47:51 ON 02 FEB 2007
D STAT QUE L125

=>